Evaluation of the Centers for Chemical Innovation (CCI) Program (2004-2016)

FINAL REPORT

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Contents

Exhibits

Acronyms and Abbreviations

Abt	Abt Associates
ACS	American Chemical Society
CAICE	Center for Aerosol Impacts on Climate and the Environment
CaSTL	Center for Chemistry at the Space-Time Limit
CCE	Center for Chemical Evolution
CCHF	Center for Selective C-H Functionalization
CCI	Centers for Chemical Innovation
C-SITS	Comparative, Short Interrupted Time Series
CENTC	Center for Enabling New Technologies through Catalysis
CHE	Division of Chemistry
CREST	Centers of Research Excellence in Science and Technology
CSMC	Center for Sustainable Materials Chemistry
CSN	Center for Sustainable Nanotechnology
CSP	Center for Sustainable Polymers
DOI	Digital Object Identifier
EAC	Evaluation & Assessment Capability
EPA	Environmental Protection Agency
ERC	Engineering Research Center
ETT	Evaluation Technical Team
GOALI	Grant Opportunities for Academic Liaison with Industry
HBCU	Historically Black Colleges and Universities
IUCRC	Industry University Cooperative Research Centers
JCR	Journal Citation Report
MPS	Mathematical & Physical Sciences Directorate
MRSEC	Materials Research Science and Engineering Center
MSI	Minority Serving Institution
NAS	National Academy of Sciences
NETE	NET ESolutions Corporation
NRC	National Research Council
NSF	National Science Foundation
OIA	National Science Foundation Office of Integrative Activities
OMB	Office of Management and Budget
PD	Program Director
PFC	Physics Frontiers Centers
PI	Principal Investigator
Postdoc	Postdoctoral researcher
RISE	Research Infrastructure for Science and Engineering
RQ	Research question
SBIR	Small Business Innovation Research
SBTTR	Small Business Technology Transfer Research
Solar	Center for Chemical Innovation in Solar Fuels
STC	Science and Technology Center

STEM	Science, Technology, Engineering, and Math
TWG	Technical Working Group
URG	Underrepresented Group
USPTO	U.S. Patent and Trademark Office

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In addition, the evaluation design and our interpretation of the findings were facilitated by the external Technical Working Group that included Professor Victor Batista, Dr. Kevin Boyack, Dr. Emilio Bunel, Dr. Daryl Chubin, Professor Melissa Hines, Dr. Gretchen Jordan, and Professor Tara Meyer. We are grateful for their guidance and feedback.

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Statement of Purpose

In 2017, NSF contracted with Abt Associates to conduct an external evaluation of the Centers for Chemical Innovation (CCI) Program, which focused on the centers funded between 2004 and 2016.[1] The evaluation focused on the contribution of the CCI Program to knowledge, workforce development, commercialization, and public outreach; the role of the center structures and operations in achieving the program goals; and the effectiveness of the two-phase funding model.

To increase the validity and completeness of the data, the evaluation utilized a mixed-methods approach that drew on the review of numerous administrative documents, surveys and interviews of CCI participants and non-participants, and an analysis of publications. The study sample included 14 centers that received only Phase I CCI awards and 9 centers that received both Phase I and Phase II CCI awards. Comparison samples of Principal Investigators on individual NSF grants funded by the Division of Chemistry and on other centers funded by NSF were used for some analyses. The study was informed by a literature review, and approved by an external Technical Working Group (TWG) and by NSF evaluation and program staff.

This report presents our evaluation findings. It can be used by NSF for planning and implementation of the CCI Program and to articulate its accomplishments to stakeholders; by CCI participants and the broader scientific community to learn from and about the program; and by program evaluators interested in learning about strategies to assess large research centers or using the data for benchmarking their studies of similar programs.

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1 Administrative records included in the study covered the period of 2004–2017; bibliometric, interview, and survey data covered the period through 2019.

Executive Summary

Introduction

The National Science Foundation (NSF) established the Centers for Chemical Innovation (CCI) Program (formerly known as Chemical Bonding Centers) in 2004 to support research focused on major, long-term challenges in fundamental chemistry. NSF envisioned that CCIs will: (1) conduct transformative research that leads to innovation and attracts broad scientific and public interest; (2) use agile structures that can quickly respond to emerging scientific opportunities; and (3) integrate research, innovation, education, inclusion of underrepresented groups, and public outreach.

The CCI Program uses a two-phase funding mechanism. In Phase I, grantees receive up to $1.8 million for three years to conduct research; contribute to the broader impact goals of NSF; and develop the infrastructure, vision, programs, and partnerships for a major research center. All grantees are eligible to apply for a Phase II award of up to $20 million over five years with a possibility of a competitive renewal of the same size and duration. In Phase II, grantees are expected to implement the vision developed in the first phase.

In 2017, NSF contracted with Abt Associates to conduct an evaluation of the CCI Program. The sample included the 14 centers that received Phase I awards only and the 9 centers that received both Phase I and Phase II awards through 2016, but the evaluation focused particularly on the Phase II awards, which are listed below.

- Center for Enabling New Technologies through Catalysis (CENTC), led by the University of Washington
- Center for Chemical Innovation in Solar Fuels (Solar), led by the California Institute of Technology
- Center for Chemistry at the Space-Time Limit (CaSTL), led by the University of California-Irvine
- Center for Chemical Evolution (CCE), led by the Georgia Institute of Technology
- Center for Sustainable Materials Chemistry (CSMC), led by Oregon State University
- Center for Selective C-H Functionalization (CCHF), led by Emory University
- Center for Aerosol Impacts on Climate and the Environment (CAICE), led by the University of California-San Diego
- Center for Sustainable Polymers (CSP), led by the University of Minnesota-Twin Cities
- Center for Sustainable Nanotechnology (CSN), led by the University of Wisconsin-Madison

To facilitate our understanding of the CCI Program and to identify linkages between program inputs, processes, and outcomes we developed a logic model, as shown in Exhibit E1.

Exhibit E1: CCI Program Logic Model

Phase I Awards

INPUTS

Submission of preliminary and full Phase I proposals with
Focus on major, long-term fundamental challenges in chemistry

Funding
NSF Funding (up to $1.8 M for 3 years)

Encouraged by NSF but not required

Collaborations with
- Academic institutions
- Non-profit, non-academic organizations
- Industry
- Government laboratories
- International organizations

ACTIVITIES

Develop management structures for major research center
- Strategic planning*
- Cross-collaboration data management*

Engage in fundamental chemical research and disseminate findings

Pilot broader impact activities
- Innovation
- Higher education and professional development
- Broadening participation of underrepresented groups
- Informal science communication

OUTPUTS AND OUTCOMES

- Strategic plan* and vision for Phase II
- Cross-collaboration data management plan*
- New collaborations
- Enhanced team integration and productivity (synergy)
- New research directions
- High-impact publications
- Licenses, invention disclosures, patent applications
- Higher quality training and professional development opportunities for students and postdocs
- New tools, materials, technologies, methodologies, theory
- Improved public understanding and appreciation of chemistry
- Leveraged funding
- Phase II award

Phase II Awards

INPUTS

Successful Phase I Awardees Submit Full Phase II Proposals
- Center overview & management plan
- Results of prior CCI support
- Proposed CCI research

Funding & Advisory
- NSF Funding (up to $4 M per year for 5 years)

Encouraged by NSF but not required

Collaborations with
- Academic institutions
- Non-profit, non-academic organizations
- Industry
- Government laboratories
- International organizations

ACTIVITIES

Engage in fundamental chemistry research to address challenges of large scope and impact

Implement strategic center-scale activities in broader impact areas:
- Innovation
- Higher education and professional development
- Broadening participation of URGS
- Informal science communication

Disseminate research via:
- Papers
- Articles/books
- Conference
- Patent applications
- Social media or other informal channels

OUTPUTS AND OUTCOMES

- Advances in fundamental chemistry
- High-impact publications
- Licenses, inventions, patents, and start-up companies
- New tools, materials, technologies, methodologies, theory
- New educational, professional development, and retention programs
- Enhanced professional reputation and visibility
- Leveraged funding
- Knowledge of how to run large centers
- New and sustainable strategies and partnerships to increase public education and participation of URGs in chemistry
- Sustainable partnerships and teams
- New research directions
- Enhanced economic competitiveness and innovation
- Improved public understanding and appreciation of chemistry
- Better trained students and postdocs
- More underrepresented groups involved in chemical research

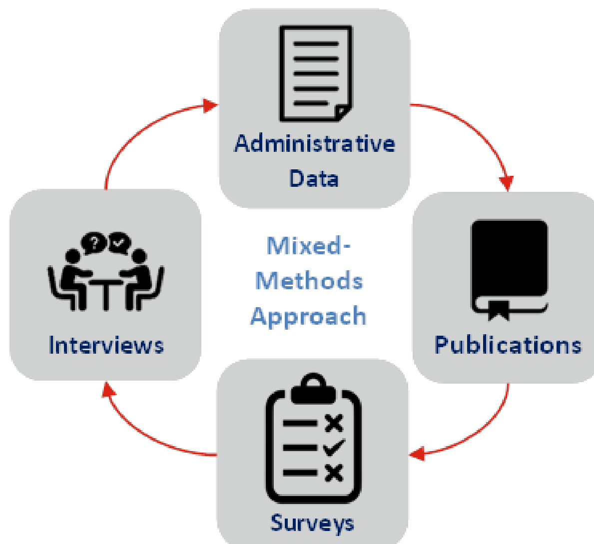
Indicates an activity or output that was not included across all program solicitations.

The evaluation addressed five broad research questions:[2]

1	**What are the important contributions of the CCI Program to our current understanding of fundamental chemistry?[3,4]**
2	**How successful have the CCI centers been at transferring their basic research results into societal or economic benefits (innovation)?**
3	**What are the contributions of the CCI Program in the areas of workforce development (education and professional development), broadening participation, and informal science communication?**
4	**How effective are the center structures and operations in achieving the program's goals?**
5	**How effective is the two-phase funding models for the CCI program?**

We used a **mixed-methods approach** to answer these questions, which included four components:

- Coding and analysis of **administrative data** collected from annual reports, grant proposals, CCI websites, site visit reports, funding and oversight memoranda, internal interim reviews, and review analyses.
- Analysis of **publications** by Principal Investigators (PIs) and Co-Investigators on CCI grants as well as on individual investigator grants funded by NSF's Division of Chemistry.
- **Surveys** of CCI PIs and Co-Investigators[5] and of graduate students, and postdoctoral researchers (postdocs).
- **Interviews** with CCI PIs, Co-Investigators, Managing Directors, and Industry Partners; Site Visitors; PIs for other NSF centers; and NSF staff.



2 Additional sub-questions for each of the broad question are addressed in the main report.

3 The first question was originally formulated as: "What are the impacts of the CCI Program on our current understanding of fundamental chemistry?" The question was revised since a comparison group is not available to evaluate program impact.

4 We were not able to assess the scientific advances in fundamental chemistry. Instead, this question focused on the productivity and influence of scientific research, the ways in which CCIs demonstrated leadership in their field and responsiveness to new developments, and how the research community benefited from the CCIs.

5 This group included all individuals who had the following titles in CCI annual reports: Primary PI, Program Director (PD)/PI, Co-PD/PI, Co-Investigator, or Senior Personnel. Additionally, for one center that had two participants listed in these roles, we also included nine individuals listed as faculty members and identified by NSF as primary investigators.

Data Collection and Analysis

Administrative Data. We reviewed and coded all available administrative records for the Phase II awards (approximately 300 documents). The information included management structure, activities, participants, accomplishments, and challenges. To retrieve these data, we combined a semi-automated scraping procedure for standardized data with manual coding for open-ended data. Based on grant proposals and annual reports, we compiled accomplishment profiles for all nine Phase II centers.

Publications. We identified 338 CCI senior researchers who participated in Phase I and Phase II centers in 2004–2016 and a comparison group of 500 NSF PIs on individual investigator grants funded by the Division of Chemistry during the same period. We matched the names of the researchers in each group to Scopus author profiles, and identified approximately 85,000 CCI and 130,000 comparison investigator publications.[6] To obtain publications that resulted from CCI funding, we queried Scopus and Web of Science databases for references to CCI grant numbers, which resulted in 2,054 publications. We then used a comparative short interrupted time series model to examine publication and citation trends for the CCI and the comparison groups.

Surveys. We administered online surveys to CCI PIs, Co-Investigators, graduate students, and postdocs who participated in the program in recent years.[7] The samples included 217 PIs/Co-Investigators and 793 graduate students/postdocs. The survey response rates for those with active email addresses were 63 percent and 52 percent, respectively. Survey responses were weighted on the available characteristics to adjust for possible non-response bias. The survey explored the characteristics of research projects, collaborations, student experiences, benefits and challenges of participation, strengths and limitations of the two-phase model, and other topics pertinent to the evaluation questions.

Interviews. We conducted 49 interviews with the following groups: Phase II Managing Directors (n=9), Phase II PIs (n=8), Phase II Co-Investigators (n=4), Industry Partners (n=4), NSF staff (n=7),[8] Site Visitors responsible for CCI oversight (n=9), and PIs on non-CCI centers (n=8). In interviews with CCI participants, we discussed the accomplishments of their centers, strengths and weaknesses of the center structure and the two-phase funding model, challenges associated with running or being part of the center, the most effective center components, features of good partnerships, and benefits of CCIs to industry. External perspective on the CCI program was explored in NSF and Site Visitor interviews. Finally, we collected contextual data on the center model from PIs on non-CCI centers funded by NSF. We used *NVivo* software to code and analyze interview data.

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6 This number represents every record associated with these investigators available in Scopus through early 2019, including peer reviewed articles, books, and conference papers.

7 Samples were limited to PIs and Co-Investigators included in annual reports between 2012–2013 and 2016–2017 and to graduate students and postdocs between 2014–2015 and 2016–2017.

8 The views provided by NSF staff in interviews reflect their individual positions only.

Study Limitations

The study has several limitations that may affect the validity of the data and/or their interpretation, most of which are common for evaluations of research programs.

- **Lack of causal attribution:** We were unable to definitively attribute changes in activities or outcomes to CCI funding because the study was observational rather than experimental.
- **Inability to examine long-term outcomes:** All of the Phase II centers are either still active or only recently completed their funding. Consequently, it is too early to measure the longer-term contribution of CCIs to the field, economic and societal benefits, and career paths of participants beyond the immediate next step.
- **Inability to answer all sub-questions:** We were unable to address some of the questions of interest to NSF due to the lack of measures and/or data.
- **Inconsistency and incompleteness of the administrative records:** The data included in these documents were often inconsistent across the centers and the years within the center, making it challenging to track activities and external perspective on the centers over time.
- **Author disambiguation:** It was not always possible to distinguish publication records for multiple researchers with the same name.
- **Identifying publications attributable to CCI funding:** Some publications listed in annual reports could not be matched to the Scopus or Web of Science databases.[9]
- **Potential for social desirability and recall biases:** Survey and interview respondents may have exaggerated their accomplishments and/or minimized challenges. Furthermore, activities that took place several years ago may have been difficult to recall accurately.
- **Limited and suboptimal time for data collection:** Due to the delays in obtaining OMB clearance, we had to field the surveys during the summer months and limit the duration of the data collection.
- **Small sample size of the interview data:** Interview data collected from small samples of respondents may not be representative. Further, to protect respondent anonymity, we chose to exclude from the report the information that could not be masked.

[9] NSF changed annual reporting instructions after the evaluation reference period to require centers to list DOIs and publication status for all publications, which will make it easier to match annual report publications to bibliometric databases in the future.

Findings and Conclusions

Research Question 1: What are the important contributions of the CCI Program to our current understanding of fundamental chemistry?

Productivity and influence of the scientific research

- For all CCI investigators, the total number of publications increased over the first three years after the award, from 10 to 12 papers per year per investigator.
- Comparison group productivity was significantly lower, at 8 papers per year per investigator three years after award.
- Total productivity of Phase II investigators exceeded the trend established in the pre-award period and outpaced both Phase I-only and comparison groups.
- On average, CCI investigators were more highly cited than comparison investigators, both before and after the award.
- By the end of year 3 of the Phase II award, CCI centers published an average of 26 papers per year across all investigators, a three-fold increase from the end of Phase I. In total, CCIs Phase I and Phase II centers published 2,054 papers acknowledging CCI support through early 2019.
- CCI-acknowledging papers appeared in higher-impact journals than a random sample of comparison investigator papers.
- In the survey, CCI PIs and Co-Investigators confirmed that CCI participation increased publication productivity, the range of the journals in which the papers were published, and the journal quality.
- CCIs reported numerous scientific accomplishments in annual reports and renewal proposals, but we were unable to judge their importance or influence on the field due to their highly technical nature.

Leadership in the field and responsiveness to new developments

- The majority of investigators surveyed indicated that their research addressed a major challenge in chemistry/an important societal problem, had the potential to radically change our understanding of an important concept, and was interdisciplinary and high-risk.
- The study provided strong evidence that the program offered many benefits to researchers affiliated with the centers. Nearly all CCI PIs and Co-Investigators reported that participating in the center helped them recruit better students and postdocs, obtain additional funding, access institutional resources, and broaden their research program.
- In interviews and in the survey CCI participants reported that the center model enabled them to more quickly respond to scientific developments by disseminating information within their network, drawing on multi-disciplinary expertise, and quickly marshalling resources.
- The CCI Program funded well-known scientists, whose standing was further enhanced through participation in the program. CCI participants served as advisors, editors, and reviewers; and received numerous awards, prizes, and other honors, including two MacArthur Fellowships, known as “genius awards” (Exhibit E2).

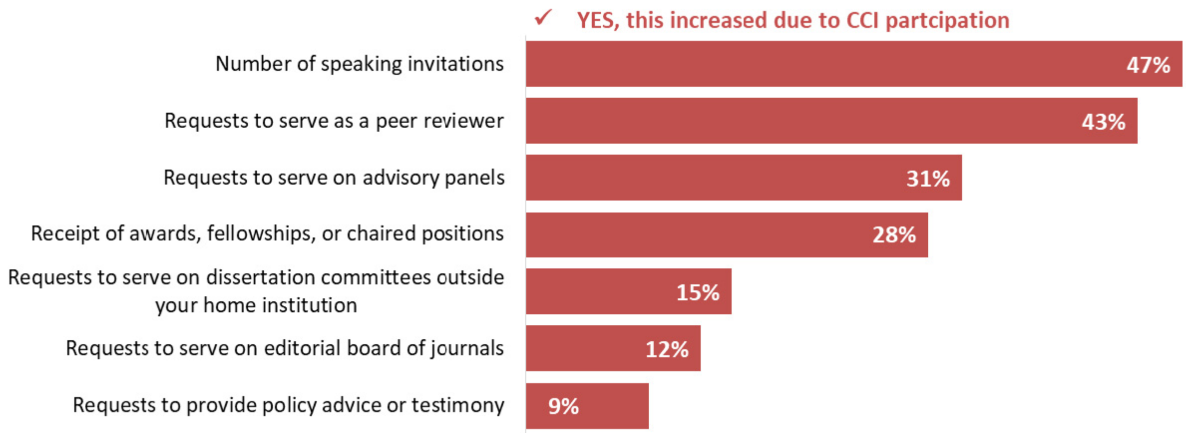
Benefits to the chemistry research community

- The equipment, facilities, and tools developed by CCIs also benefited unaffiliated scientists. In addition, CCIs produced a cohort of well-trained and well-rounded young scientists and helped inform the public about the importance of scientific research.

Recommendation for Research Question 1:

- NSF could consider engaging an external expert panel or a similar entity to further evaluate the scientific contributions of CCIs and their influence on the research community.

Exhibit E2: Percent of CCI PIs and Co-Investigators Reporting Improved Professional Outcomes in the Survey



Research Question 2: How successful have the CCI centers been at transferring their basic research results into societal or economic benefits (innovation)?

- CCIs developed numerous ties to academic institutions, industrial firms, nonprofits, national laboratories, federal agencies, schools, and professional associations. These partnerships ranged from collaborative projects, to financial and in-kind support, to venues for student training and public outreach. Phase II centers had an average 24 partners, with one reporting 43 partners.
- CCIs are commercializing their research findings, as evidenced by invention disclosures, licenses, patents, and start-up companies. Examples of products being developed by these companies include more degradable plastics, energy storage devices, polymer platforms, and instrumentation to assess atmospheric aerosols.
- Benefits of CCIs to commercial partners reported by center participants included improved access to ideas, products, processes, and people; a reduction in environmental impacts; and the ability to meet regulatory requirements.
- CCIs also contributed to commercialization indirectly through their workforce development efforts. Approximately one-third of graduate students and one-quarter of postdocs reported in the survey that a position in industry became their career goal after joining a CCI. Furthermore, just under one-third of CCI investigators also reported an increased interest in commercialization. Industry representatives confirmed in interviews that CCIs bring together the academic and industry communities.

Research Question 3:
What are the contributions of the CCI Program in the areas of workforce development (education and professional development), broadening participation, and informal science communication?

Workforce Development

- CCIs launched numerous courses, seminars, and research experiences for students and postdocs. In addition, they offered a wide range of opportunities to develop transferrable skills, such as leadership, management, communication, and mentoring.
- Participation in and satisfaction with many of the activities offered by CCIs was very high (Exhibit E3). However, less than 50 percent of students and postdocs reported supervising students, applying for grants and fellowships, visiting other research labs, teaching, and entrepreneurship. At the same time, less than 30 percent indicated that they were well prepared to teach, write proposals, and work outside of academia – the very same skills that these activities could improve.
- Many CCI students and postdocs had multiple mentors and about a third had an opportunity to spend time in partner laboratories, which was viewed as a valuable experience. Three-quarters reported having a collaboration with researchers outside of their institution (Exhibit E3).
- The vast majority graduate students and postdocs reported that participating in CCI was advantageous to their careers. They felt prepared to conduct research, work in teams, think critically about problems, communicate, and serve as mentors. Being part of CCI also reportedly improved access to job opportunities.
- CCI participation influenced career choices of graduate students and postdocs, including the type of institution, research problem, and discipline. Of the students who had left CCIs and responded to the survey, 44 percent reporting having a position in academia, 29 percent in industry, and 12 percent in government.
- CCI faculty believed that the centers brought about improvements in the quality of education in chemistry and helped students and postdocs obtain their next position.

Broadening Participation

- CCIs developed many strategies to broaden participation of underrepresented groups in science. These included partnerships with relevant educational institutions and professional societies, programs targeting K-12 and college students, and mentorship/peer support for students who joined the centers.
- Most CCI investigators articulated in the survey that the center activities related to broadening participation increased the diversity of their own laboratory and institution and contributed to the success of their center.
- Based on the survey data, CCIs had higher representation of racial and ethnic minorities and similar representation of women among students and postdocs to the national average in chemistry.

Informal Science Communication

- CCIs launched numerous public outreach efforts, such as science festivals and fairs, portable experiments, poster competitions, museum exhibits, and public lectures. To reach the broadest swath of society possible, the centers took advantage of a range of venues, from cafes to classrooms. Some of the products and programs developed by CCIs reached thousands of people.

- Virtually all PIs and Co-Investigators reported that their outreach efforts contributed to the success of the center and increased the interest in and understanding of chemistry among the public.

Sustainability of Broader Impact Efforts

- Half or more of the CCI PIs and Co-Investigators surveyed believed that many of the broader impact programs were sustainable. However, in interviews PIs and Managing Directors indicated that the legacies of CCIs were more likely to include collaborations, discoveries, companies, and scientists trained.

Recommendation for Research Question 3:

- CCIs should consider encouraging more students and postdocs to participate in teaching, grant writing, entrepreneurship, and visits to partner institutions. Less than 50 percent of these researchers took advantage of these opportunities at the centers, while many also reported that they lacked the skills these very same activities would develop.

Exhibit E3: CCI Students and Postdocs were Satisfied with Many Professional Development Opportunities Available to Them

Research Question 4: How effective are the center structures and operations in achieving the program's goals?

- CCI PIs were praised for their personal dedication to the centers, ability to clearly articulate expectations and keep participants engaged, and their commitment to transparency and shared governance.
- Managing Directors play an important role in running Phase II centers by helping run the operations of the center and sharing best practices and lessons learned, and generally facilitating program cohesion. Two Managing Directors argued that it would be helpful to have this type of position in Phase I to help design and prepare the larger center.
- The long duration and large budgets of the centers offered participants an opportunity to find their niche and lay the theoretical and/or experimental foundation to tackle complex problems.
- One of the strengths of the CCIs is their flexibility – both in abandoning unproductive directions and in rapidly marshaling resources and expertise to respond to new developments. CCIs also have the "luxury" to explore scientific problems that a single PI would consider too risky or costly.
- Retention in the centers was high – 95 percent of investigators remained affiliated for at least 2 years and 54 percent for at least 7 years.
- Both CCI investigators and Site Visitors highlighted the collaborative culture as the major strengths of the centers. Consistently, the analysis of publications by CCI investigators showed a dramatic increase in the level of co-authorships during the grant, from 6–7 percent to 23–27 percent.
- In the survey, the vast majority of investigators were satisfied with the intellectual contribution of partners, communication tools, data sharing, frequency and productivity of meetings, distribution of resources, and the program overall. While some challenges were reported in these areas, these were mostly resolved.
- CCI PIs said that it was sometimes challenging to keep all participants engaged and focused on the mission of the center. PIs had to remove partners who were either not collaborative or no longer contributed to the mission of the centers, and found this a difficult responsibility for which they were not necessarily prepared.
- Some Site Visitors, NSF staff, and CCI investigators thought that publication productivity of CCIs was lower than for other programs. These concerns were not borne out in the bibliometric analysis, which showed that CCI PIs published more papers per year than their peers on individual NSF grants.

Recommendations for Research Question 4:

- Given the extensive evidence on the many benefits of the center mechanism, NSF should continue to invest in this strategy.
- NSF could consider optional funding for a Managing Director position in Phase I or other creative solutions to project management. This would allow PIs to focus on the scientific mission and partnerships of the larger center.

Research Question 5:
How effective is the two-phase funding model for the CCI Program?

- The model was strongly endorsed by the researchers who participated in both phases of the program. CCI PIs and Co-Investigators reported that the model allowed them to refine their research goals and approach, pilot activities and programs, select the right partners, develop and test center policies and procedures, and determine if the team science experience was a good fit for them. Survey respondents also believed that Phase I enables NSF to select better Phase II centers, thus reducing the risks associated with large investment (Exhibit E4).
- The main limitations of the model that emerged from the study were the opportunity cost and effort for unsuccessful Phase I groups, the risk of excluding good Phase I centers, the lack of flexibility in the funding amount for Phase II, and the need to invest time in writing Phase II proposals.

Recommendation for Research Question 5:

- NSF should continue supporting the two-phase funding mechanism. The two-phase approach was strongly endorsed by most participating researchers, particularly those that were awarded Phase II awards.

Exhibit E4: The Advantages of the Two-Phase Model

Summary of Findings

In summary, the evaluation has yielded substantial information about the operation and outcomes of the CCI Program. We found that the majority of researchers at all career levels were very satisfied with their experiences and explicitly linked their time at CCIs to many important professional outcomes. Program participants were also in agreement about the advantages of the center model in general and the two-phase mechanism specifically, and endorsed this funding strategy for future centers. The CCI community outperformed the individual grant investigators in the number of publications, citation impact, and journal quality. Finally, CCIs launched numerous programs to support workforce development, public education, and participation of underrepresented minorities in STEM. While the evaluation relied heavily on self-reported data and was not designed to establish causality, the breadth and consistency of evidence allows us to conclude that the CCI Program is meeting its intended goals.

Chapter 1: Introduction

The Centers for Chemical Innovation Program

In 2003, the National Science Foundation (NSF) issued a report that summarized the findings from a Workshop on New Mechanisms for Support of High-Risk and Unconventional Research in Chemistry. The report recommended the introduction of a center-based funding mechanism specifically designed to support high-risk, collaborative research in chemistry, which could lead to groundbreaking results.[10] NSF launched the Centers for Chemical Innovation (CCI) Program (formerly known as Chemical Bonding Centers) the following year. The goal of the CCI Program is to "support research centers focused on major, long-term fundamental chemical research challenges" and to "integrate research, innovation, education, broadening participation, and informal science communication."[11]

The program uses a two-phase funding strategy. Phase I centers receive $1.8 million in support for three years.[12] During the funding period, grantees are expected to conduct research and training activities; and to lay the foundation for a larger center by developing partnerships, infrastructure, and programs. At the end of Phase I, the centers are eligible to apply for a Phase II grant of up to $20 million over five years, with a possibility of a competitive renewal of the same size and duration.[13] Phase II centers build on and expand the activities begun in the first phase, but have the flexibility to change the research direction, infrastructure, people, and programs.

To facilitate our understanding of the CCI Program and to identify links among program inputs, processes, and outcomes, we developed the program logic model shown in Exhibit 1. In brief, NSF funding, pre-existing collaborations, and grant applications represent inputs in the context of the CCI Program. Once the awards are made, grantees are expected to engage in various activities to accomplish CCI goals, such as developing an infrastructure for a research center, conducting and disseminating research, and advancing NSF's broader impact goals. The logic model postulates that these activities will in turn lead to various results (outputs and outcomes), such as strategic and management plans for the centers, training and research programs, and new tools and discoveries. These accomplishments are anticipated within the short- and medium-term after the program launch – within 15 years – to align with the timing of the evaluation study relative to the establishment of the first cohort of Phase I grants. The logic model guided our literature search and the design of the data collection approaches and tools based on this body of evidence.

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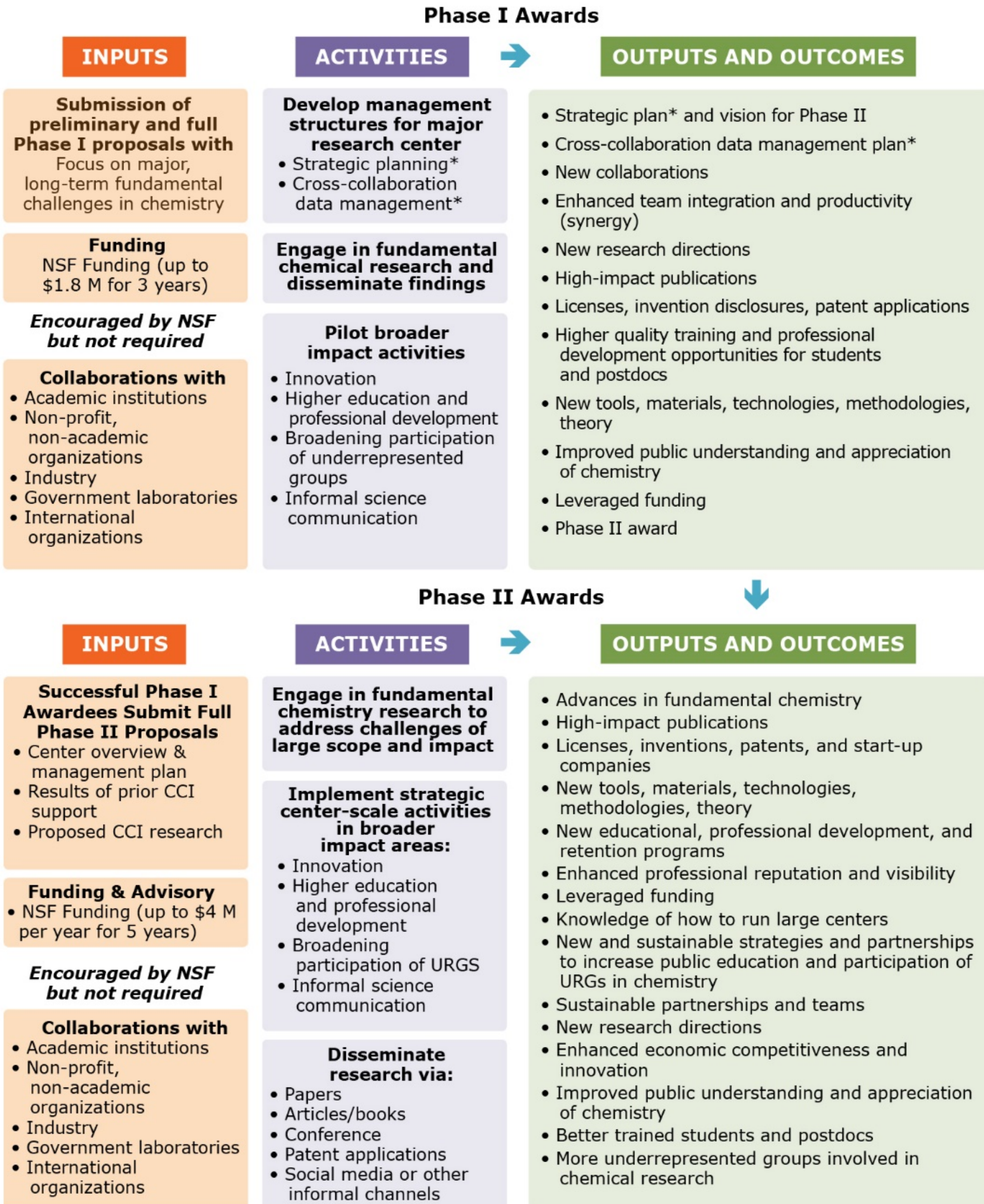
10 https://www.scribd.com/document/996025/National-Science-Foundation-nsfgmwfinal.

11 https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=13635.

12 https://www.nsf.gov/pubs/2017/nsf17564/nsf17564.pdf.

13 Phase I centers only have one opportunity to compete for a Phase II award.

Exhibit 1: CCI Program Logic Model



Indicates an activity or output that was not included across all program solicitations.

While the evaluation examines activities and outcomes of both Phase I and Phase II centers, it focuses primarily on the nine Phase II centers funded through 2016:[14]

- Center for Enabling New Technologies through Catalysis (CENTC), led by the University of Washington
- Center for Chemical Innovation in Solar Fuels (Solar), led by the California Institute of Technology
- Center for Chemistry at the Space-Time Limit (CaSTL), led by the University of California-Irvine
- Center for Chemical Evolution (CCE), led by the Georgia Institute of Technology
- Center for Sustainable Materials Chemistry (CSMC), led by Oregon State University
- Center for Selective C-H Functionalization (CCHF), led by Emory University
- Center for Aerosol Impacts on Climate and the Environment (CAICE), led by the University of California-San Diego
- Center for Sustainable Polymers (CSP), led by the University of Minnesota-Twin Cities
- Center for Sustainable Nanotechnology (CSN), led by the University of Wisconsin-Madison

Abt Associates Evaluation

In 2017, NSF contracted with Abt Associates (Abt) to conduct an external evaluation of the CCI Program, which covered the period from program establishment in 2004 through 2019.[15] The CCI Program is a significant investment for NSF and it is critical that the findings of the evaluation are as widely used as possible. This report, which presents our evaluation findings, can be used by NSF for planning and implementation of the CCI Program and to articulate its accomplishments to stakeholders, by CCI participants and the broader scientific community to learn from and about the program, and by program evaluators interested in learning about strategies to assess large research centers or using the data for benchmarking their studies of similar programs.

The evaluation aimed to address 5 primary research questions (RQs) and 14 sub-questions that are both formative and summative in nature. We made minor changes to the wording of original RQs 1, 1.1, 1.4, 2.1, and 4.2 to ensure they could be feasibly answered using the proposed design and available data. First, we removed the term “impact,” which would require an experimental or quasi-experimental design not practical for this program. Second, we removed the wording “to what extent” in instances when reliable quantification did not seem possible. These changes are indicated in the footnotes. The final set of RQs that guided the study was as follows:

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[14] The study sample included 14 centers that received only Phase I awards and 9 centers that received Phase I and Phase II awards. This represented all centers with documentation available through August 2018. Information about the Phase II centers can be found here: [NSF CCI](#).

[15] Administrative records included in the study covered the period of 2004–2017; bibliometric, interview, and survey data covered the period through 2019.

Research Question 1: What are the important contributions of the CCI Program to our current understanding of fundamental chemistry?[16]

1.1 What is the evidence of productivity and influence of the scientific research?[17]

1.2 To what extent and in what ways have the CCI centers demonstrated both leadership in their field and responsiveness to developments in their field?

1.3 Does the center mechanism of operation contribute to the research achievements of the centers?

1.4 In what ways has the chemistry research community benefited from the CCI centers?[18]

Research Question 2: How successful have the CCI centers been at transferring their basic research results into societal or economic benefits (innovation)?

2.1 In what ways have the research findings and other center achievements contributed to societal and economic benefits?[19]

2.2 In what ways have the CCIs developed partnerships to engage in technology transfer, to commercialize technology, or for other societal benefit?

Research Question 3: What are the contributions of the CCI Program in the areas of workforce development (education and professional development), broadening participation, and informal science communication?

3.1 What are the most important impacts of the CCIs in these three areas and how was this made possible (or enhanced) by the center mechanism of operation?

3.2 To what extent and in what ways are the CCIs providing leadership in these three broader impact areas?

3.3 To what extent and in what ways have the CCIs contributed to sustained, institutionalized change in these three broader impact areas?

Research Question 4: How effective are the center structures and operations in achieving the program's goals?

4.1 What are some of the most effective center management strategies, and how are they adapted to their particular situations, in promoting (1) transformative outcomes, (2) enhanced team integration and augmented productivity (synergy), (3) higher quality training opportunities for students and postdocs, (4) increased diversity, and (5) improved public understanding and appreciation of chemistry?

4.2 To what extent and in what ways have the CCIs influenced collaborations among center participants?[20]

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16 RQ 1 was originally specified as: "What are the impacts of the CCI Program on our current understanding of fundamental chemistry?" We were not able to assess the scientific advances in fundamental chemistry. Instead, this question focused on the subquestions.

17 RQ 1.1 was originally specified as: "What is the evidence of productivity and impact of the scientific research?"

18 RQ 1.4 was originally specified as: "To what extent and in what ways has the chemistry research community benefited from the CCI centers?"

19 RQ 2.1 was originally specified as: "To what extent and in what ways have the research findings and other center achievements contributed to societal and economic benefits?"

4.3 To what extent and in what ways have the CCIs made use of tools and communication to facilitate collaboration?

Research Question 5: How effective is the two-phase funding model for the CCI Program?

5.1 What are the strengths and weaknesses of the two-phase award process?

5.2 What is the value of the Phase I award experience for the awardees?

The evaluation utilized a mixed-methods approach, which included the following components:

- Coding and analysis of administrative records – to document program accomplishments and views on progress from peers responsible for external oversight;
- Analysis of publication records (bibliometrics) of CCI Principal Investigators (PIs) and Co-Investigators, as well as of PIs on individual-investigator grants funded by NSF's Division of Chemistry (CHE) – to measure research productivity and reach;
- Surveys of PIs, Co-Investigators, graduate students, and postdoctoral researchers (postdocs) – to understand the role of the center in research, collaboration, workforce development, and other broader impacts; to assess grantee satisfaction with the center's structure and a two-phase funding model; and to describe the challenges encountered; and
- Interviews with CCI PIs and Co-Investigators, Industry Partners, Site Visitors, and PIs on other NSF centers – to further explore and validate the themes emerging from surveys and administrative documents, and to obtain context on non-CCI center programs.

The remainder of this report is organized as follows. Chapter 2 includes a description of the methods and study limitations, Chapters 3–7 respond to each RQ posed by NSF, and Chapter 8 contains conclusions and recommendations.

The report also includes several appendices: Appendix A – a review of the literature, Appendix B – the evaluation framework, Appendix C – the list of patents awarded to CCIs, Appendix D – element codes for the comparison programs included in this study, Appendix E – data collection instruments, Appendix F – sensitivity analyses for publication data, Appendix G– a list of grand challenges, Appendices H and I – survey data for CCI PIs/Co-Investigators and graduate students/postdocs, Appendix J – supplemental tables corresponding to the charts included in Chapters 3–7, and Appendix K – chord diagrams of publication networks for additional CCIs.

[20] RQ 4.2 was originally specified as: "To what extent and in what ways have the CCIs influenced and impacted collaborations among center participants?"

Chapter 2: Methodology

In this chapter we describe our data collection and analysis strategies, oversight and feedback provided by NSF and external experts during the course of the study, and the challenges and limitations of the study.

Evaluation Framework

To inform the evaluation design and data collections/analysis strategies, we conducted a review of publications, agency reports, evaluation reports, national surveys, funding opportunity announcements, and CCI Program documents. The review focused on topics pertinent to the study, including productivity and influence of scientific research, societal and economic benefits of research, broader impacts as defined by NSF and the research centers, and the two-phase approach to funding research programs. The focus of the review was on definitions and measurements of CCI-relevant constructs. Appendix A summarizes the information that emerged from the review.

Next, we developed an evaluation framework, which identified indicators for each RQ and sub-question (Appendix B).[21] These indicators were either reported in the literature or were developed by our team based on the literature and on our own experience evaluating research programs. Once the set of indicators was established, we determined where and how these data would be collected and analyzed, and if a comparison group was available and appropriate. This systematic approach yielded a document that formed the foundation of the study. The literature review and the evaluation framework were reviewed and approved by NSF.

Data Collection

Exhibit 2 displays the data collection methods used to respond to each of the five RQs and 14 sub-questions. As the reader can see, we drew on multiple data sources in each case. This is an important advantage of a mixed-methods evaluation because (as discussed below) each method has limitations, and relying on multiple sources for evidence helps produce more complete and reliable data.

Exhibit 2: Research Question and Sub-Questions Linked to Data Collection Strategies

Research Questions and Sub-Questions	Publication Data	CCI PI and Co-Investigator Surveys	CCI Graduate Student and Postdoc Surveys	CCI PI and Managing Director Interviews	Industry Partner Interviews	Site Visitor and NSF Staff Interviews	Comparison Center PI Interviews	Coding of CCI Administrative Data
1. What are the important contributions of the CCI Program to our current understanding of fundamental chemistry?	✓	✓		✓		✓	✓	✓
1.1 What is the evidence of productivity and influence of the scientific research?	✓	✓		✓				✓

21 Within the evaluation framework, we list the full set of indicators relevant to each RQ and sub-question, but since many indicators were relevant to multiple questions, we present the findings for each indicator under the most relevant sub-question.

Research Questions and Sub-Questions	Publication Data	CCI PI and Co-Investigator Surveys	CCI Graduate Student and Postdoc Surveys	CCI PI and Managing Director Interviews	Industry Partner Interviews	Site Visitor and NSF Staff Interviews	Comparison Center PI Interviews	Coding of CCI Administrative Data
1.2 To what extent and in what ways have the CCI centers demonstrated both leadership in their field and responsiveness to developments in their field?		✓		✓		✓		
1.3 Does the center mechanism of operation contribute to the research achievements of the centers?	✓	✓		✓		✓	✓	
1.4 In what ways has the chemistry research community benefited from the CCI centers?		✓		✓	✓	✓		✓
2. How successful have the CCI centers been at transferring their basic research results into societal or economic benefits (innovation)?		✓		✓	✓	✓		✓
2.1 In what ways have the research findings and other center achievements contributed to societal and economic benefits?		✓			✓	✓		✓
2.2. In what ways have the CCIs developed partnerships to engage in technology transfer, to commercialize technology, or other societal benefit?		✓		✓	✓			✓
3. What are the contributions of the CCI Program in the areas of workforce development, broadening participation, and informal science communication?		✓	✓	✓		✓		✓
3.1. What are the most important impacts of the CCIs in these three areas and how was this made possible (or enhanced) by the center mechanism?		✓	✓	✓		✓		✓
3.2 To what extent and in what ways are the CCIs providing leadership in these three broader impact areas?		✓	✓					✓
3.3 To what extent and in what ways have the CCIs contributed to sustained, institutionalized change in these three broader impact areas?				✓				✓
4. How effective are the center structures and operations in achieving the program's goals?	✓	✓	✓	✓	✓	✓	✓	✓
4.1 What are some of the most effective center management strategies, and how are they adapted to their particular situations, in promoting broader impacts?		✓	✓	✓	✓	✓	✓	✓
4.2 To what extent and in what ways have the CCIs influenced collaborations among center participants?	✓	✓			✓	✓		✓
4.3 To what extent and in what ways have the CCIs made use of tools and communication to facilitate collaboration?		✓				✓		✓
5. How effective is the two-phase funding model for the CCI Program?		✓		✓	✓	✓	✓	
5.1. What are the strengths and weaknesses of the two-phase award process?		✓		✓		✓	✓	
5.2. What is the value of the Phase I award experience for the awardees?		✓		✓		✓		

Administrative Data

We reviewed all available administrative records for the Phase II awards (Exhibit 3).[22, 23] These documents were used to capture the management structure, accomplishments and outputs, activities, participants and collaborations, and challenges reported by the grantees and from external points of view. We used the list of patents from annual reports to manually query the U.S. Patent and Trademark Office (USPTO) database and *Google Patents*. All awarded patents returned were searched for acknowledgment of CCI funding. Appendix C includes the list of CCI patents cited in the annual reports.

Exhibit 3: Counts of Documents by Type

Type of Document	Document Description	Count[a]
Center-Generated Administrative Records		
Phase II annual reports	Centers are required to submit annual reports (using the NSF-recommended Progress Report format, which changed over time) with information on key scientific outcomes, accomplishments, products, participants and other collaborating organizations, impacts, and changes/problems during the budget period or year. The annual report also describes plans for the subsequent budget period or year.	58
Attachments to annual reports	Centers may append other documents to their annual reports, such as information about broader impacts, outreach and diversity, conference papers, and other research activities.	139
Phase II proposals (initial and renewal)	Centers submit a Phase II proposal at the end of their Phase I award or first Phase II award. Phase II proposals are reviewed using a combination of *ad hoc* review and a reverse site visit, during which center researchers have the opportunity to present their Phase I (or first Phase II) accomplishments and Phase II (or second Phase II) plans to an expert panel of reviewers and NSF staff.	17
Websites	Each Phase II center developed a center-based website to present their key research themes, team members, key activities, resources, and accomplishments for their center.	9
Non-Center-Generated Administrative Records		
Site visit reports	Site visits and reverse site visits are scheduled oversight events (e.g., in the second, fourth, and seventh years of Phase II awards; and in the Phase II proposal/renewal competition) in which a panel of experts and NSF staff review centers' strategic plans and assess their work to date. Site visit reports provide feedback on such areas as intellectual merit, broader impacts, and CCI-specific review criteria.	22
Funding/oversight memoranda	Funding and oversight memoranda are additional reviews by NSF that document key accomplishments in research and broader impacts in the past year, funding actions, support history and plans, and program oversight.	36
Internal interim reviews	Internal interim reviews are conducted on a periodic basis by NSF staff (both inside and outside of CHE) to assess whether the centers are making sufficient scientific and technical progress.	7
Review analyses	Review analyses are written by NSF staff to justify the recommendation to either award or decline the proposal. Review analyses contain a synthesis of all external and internal reviewers' analyses and evaluations of CCI proposals against merit review criteria of intellectual merit, broader impacts, and CCI-specific review criteria.	14

[a] *Counts of documents include supplemental and other related documents.*

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22 The coding team used an automated process to pull data from annual reports from Phase I awards corresponding to the Phase II centers in order to obtain information on numbers of participants and partner organizations. No other documents were reviewed from the corresponding Phase I awards.

23 Reviewed administrative records cover CCI activities between 2004 and 2017.

Publication Data

To construct a CCI dataset, we used names of 338 senior personnel from Phase I and Phase II centers listed in annual reports for all years available at the time: 2004–2012 for Phase I and 2006–2016 for Phase II. To construct a comparison dataset, we began with all NSF grants funded by CHE between September 1, 2004 and September 15, 2016 (primary program element codes for the comparison awards are listed in Appendix D). From this list, we excluded awards with titles containing the terms *symposium*, *workshop*, *conference*, *congress*, *fellow*, or *student*; as well as awards of less than $50,000. We de-duplicated the resulting list and excluded all individuals who participated in the CCI Program. Of the remaining 2,148 PIs, we randomly sampled 500, who formed our comparison group.

We matched the names of CCI senior personnel and comparison PIs to Scopus author profiles, restricting the authors to physical sciences in an effort to eliminate multiple authors with the same name. We found that 1,096 Scopus Author identifications (IDs) corresponded to 327 unique CCI individuals.[24] We used a similar procedure for the comparison set of 500 PIs, which resulted in 1,609 Author IDs for 497 unique individuals. Using the Scopus Application Programming Interfaces licensed to NSF, we downloaded all publications corresponding to the selected profiles for these 327 CCI and 497 comparison PIs. The resulting dataset contained 84,882 CCI and 130,660 comparison investigator publications, of which 3,369 publications were present in both sets.[25] This *full dataset* was imported into a PostgreSQL database for analysis.[26]

We used two separate approaches to identify publications that resulted from CCI funding: (1) by searching for items in annual reports against Scopus and search engines, and (2) by querying Scopus and Web of Science for references to CCIs and to NSF CCI grant numbers. The latter process was far more effective and resulted in the identification of 2,054 publications acknowledging CCI support.[27,28] We refer to this dataset as *acknowledging CCI support*.

We matched journal names for publications acknowledging CCI support with the 2018 Journal Citation Report (JCR) from Web of Science. As a comparison, we randomly sampled 2,500 comparison

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24 Duplications resulted from typographical errors, use/non-use of middle initials and nicknames, and name/institution changes.

25 This number represents every record associated with these investigators available in Scopus through early 2019, including peer reviewed articles, books, and conference papers.

26 Python and SQL scripts used in data collection and analysis are archived on a public GitHub site (https://github.com/NETESOLUTIONS/ERNIE/tree/master/Scopus).

27 An additional 214 publications contained a CCI grant number, but upon investigation were determined to be referencing a different funding agency using grant numbers that overlap with CCI. For example, the National Natural Science Foundation of China awarded a grant numbered 11205189, which overlaps with the grant number for the Center for Enabling New Technologies through Catalysis Phase II renewal (1205189).

28 NSF changed annual reporting instructions after the evaluation reference period to require centers to list DOIs and publication status for all publications, which will make it easier to match annual report publications to bibliometric databases in the future.

investigator publications from five years before to five years after the comparison award date.[29] We were able to match 2,000 of the 2,500 comparison publications to the JCR.[30]

Surveys

Sample and Content

Online surveys were administered to CCI PIs, Co-Investigators, graduate students, and postdocs. The instrument contained primarily closed-ended items to reduce respondent burden, and to obtain more consistent and quantitative data. To ensure that we did not miss important information by relying on a limited number of pre-programmed answer choices, many questions included an “other” option where respondents could enter comments.

The PI/Co-Investigator survey was administered to current and former participants on all Phase I and Phase II grants awarded between 2010 and 2016, and the graduate student/postdoc survey was administered to graduate students and postdocs affiliated with Phase II grants awarded during this period. Participants were from five centers that received a Phase I grant but did not receive a Phase II award (hereafter referred to as Phase I-only awards), and nine centers that received both a Phase I grant and one or more Phase II grants (hereafter referred to as Phase I/II awards). To minimize recall bias, samples were limited to PIs and Co-Investigators who were included in annual reports between the 2012–2013 and 2016–2017 reporting years,[31] and to graduate students and postdocs who were included in annual reports between the 2014–2015 and 2016–2017 reporting years. Applying these criteria resulted in samples of 219 PIs/Co-Investigators affiliated with 14 Phase I and Phase II CCIs and 809 graduate students/postdocs affiliated with 9 Phase II CCIs.[32] The topics covered in the surveys are shown in Exhibit 4 and the survey instruments are included in Appendix E.

Exhibit 4: Topics Covered in the Surveys

Topic	CCI PIs and Co-Investigators	CCI Graduate Students and Postdocs
Characteristics of research projects	✓	
Collaborations	✓	
Benefits of participation	✓	✓
Changes in publication behavior and personal visibility	✓	
Participant satisfaction	✓	✓
Challenges of participation	✓	
Benefits and limitations of a two-phase model, and the role of Phase I	✓	

29 We limited the sampling frame to publications containing DOIs (89 percent of the total) to facilitate matching to JCR.

30 Unmatched publications were primarily conference proceedings and symposia, which are generally not indexed in JCR.

31 PIs and Co-Investigators were defined using the following roles listed in annual reports: Primary PI, Program Director (PD)/PI, Co-PD/PI, Co-Investigator, or Senior Personnel. Additionally, since one center only had two participants listed in these roles, we added nine participants listed as faculty members and identified by NSF as core collaborators.

32 We were unable to identify active email addresses for 145 graduate students/postdocs and 3 PIs/Co-Investigators, so while these individuals were included in our sample, they did not receive a copy of the survey.

Topic	CCI PIs and Co-Investigators	CCI Graduate Students and Postdocs
Research and professional development opportunities offered by CCIs		✓
Reasons for leaving CCI		✓
Career status and plans and the role of CCI		✓
Demographic characteristics		✓

Survey Administration

We extracted initial contact information from the most recent annual report in which it was available, and asked CCI PIs and Managing Directors to update the list if possible. We also attempted to identify an alternative contact through internet searches for all bounced emails, but our efforts had limited success, particularly for respondents who left academia.

Programmed surveys were subjected to two rounds of pretesting. First, researchers on our team used pre-determined testing scenarios to ensure that all skip patterns and multiple choice questions worked as intended, and all glitches were corrected. Second, the survey was sent to a small number of actual respondents. These individuals were notified that they were selected to participate in the pilot testing and were asked to provide feedback on (1) the clarity and content of the questions, (2) the ease of completing the survey, and (3) the time it took them to answer all the questions. To reduce respondent burden, these pilot testers were asked to update their previous responses as needed and to complete all new items when the final version of the survey was released to the entire population.

Prior to survey release, NSF sent an invitation email to all respondents explaining the goals of the study and introducing our team. We followed up with another email containing a unique survey link and instructions. To increase participant response rates, we asked PIs and Managing Directors to send messages to their center members encouraging them to complete the survey. In addition, four reminders were sent to all non-respondents. The survey was in the field between May and July 2019.

Survey response rates, calculated as the number of individuals who completed the survey among those who had active email addresses, were 63 percent in the PI/Co-Investigator survey and 53 percent in the student/postdoc survey. The sample sizes for each group and the number of participants who completed the survey are listed in Exhibit 5.

Exhibit 5: Survey Response Rates

Category	PI/Co-Investigator Survey	Graduate Student/ Postdoc Survey
Eligible sample size[a]	217	793
Sample with active email address (A)	214	648
Completed surveys[b] (B)	134	340
Response rate (B*100/A)	63%	53%

[a] Two PIs/Co-Investigators and 16 graduate students/postdocs in our initial sample were deemed ineligible for the survey because they were either not the person we intended to survey or they were never or only tangentially involved with a center. People responding to the graduate student/postdoc survey were also considered ineligible if their role in the center was something other than master's student, doctoral student, or postdoctoral scholar (Question 6).

[b] To be counted as complete, a respondent must have answered questions past the screener section of the survey (Question 3 in the PI/Co-Investigator survey and Question 4 in the graduate student/postdoc survey).

Interviews

Interviews were conducted with (1) CCI PIs and Managing Directors, (2) Industry Partners, (3) individuals not affiliated with CCIs who participated in site visits, (4) PIs on other NSF-funded centers, and (5) NSF CCI Program Directors and individuals in leadership positions. The topics covered with each group are included in Exhibit 6 and the interview protocols are provided in Appendix E.

Exhibit 6: Topics Included in Interviews

Topic	CCI PIs, Co-Investigators, and Managing Directors	Non-CCI Center PIs	Industry Partners	Site Visitors
Types of changes in faculty behavior due to CCI participation	✓			✓
Benefits of CCI to the scientific community, industry, and the public	✓		✓	✓
Benefits of CCI to industry partners	✓		✓	✓
Satisfaction with aspects of center management, organization, and broader impacts	✓	✓	✓	
Perspective on a two-phase versus one-phase process	✓	✓		✓
Level of pre-existing and current collaboration across partners	✓	✓	✓	✓
Evidence that CCI activities and accomplishments are sustainable	✓		✓	✓
Perceived effectiveness of management and organizational strategies	✓		✓	✓
Challenges encountered because of the center's structure	✓	✓	✓	✓

The following process was used to select interview respondents:

- We invited Managing Directors and PIs of all Phase II grants to participate in the study.
- We asked each Phase II PI to recommend one–two Industry Partners and approached at least one of these for each center.
- We chose a random selection of Co-Investigators who had been involved in a Phase II center for at least five years.[33]
- NSF prepared a list of internal staff for us to interview. These individuals were selected based on their involvement with the CCI Program and availability at the time of our visit to NSF.
- We randomly selected the Site Visitors from all participants between 2010 and 2017.
- We selected eight PIs from four non-CCI NSF center-based programs (two per program). The programs included were Science and Technology Centers (STCs), Engineering Research Centers (ERCs), Materials Research Science and Engineering Centers (MRSECs), and Physics Frontiers

[33] In two of the newer Phase II centers, no Co-Investigators had been involved with the center for more than three or four years (including their time under the Phase I award for the center), so we selected the Co-Investigators with the longest tenures in the center.

Centers (PFC). All of the centers in the sample were funded in fiscal years 2010–2016 and were still active in calendar year 2019, when the interviews were conducted.

We conducted a total of 49 interviews, broken out as follows:

- Phase II CCI PIs (8 interviews)
- Phase II CCI Managing Directors (9 interviews)
- Phase II CCI Co-Investigators (4 interviews)
- Industry Partners (4 interviews)
- NSF Staff (7 interviews)
- Site Visitors (9 interviews)
- Non-CCI Center PIs (8 interviews)

CCI PIs, Managing Directors, and Co-Investigators commented on their CCI experiences; Industry Partners reflected on their relationships with CCIs and the benefits they received from the partnership; NSF staff and Site Visitors provided external perspectives on CCI activities; and PIs of non-CCI NSF center-based programs provided perspectives on their experiences with other center-based research programs and funding models. All interviews, other than those with NSF staff, were conducted by telephone by Abt researchers with interviewing experience and an understanding of program evaluation. With respondent permission, the interviews were recorded as a back-up to the notes. The interviews occurred between May 2018 and August 2019.[34]

Regulatory Approvals

The data collection, analysis, and reporting of this material was conducted in accordance with OMB Control No. 3145-0215. The study plan and instruments were reviewed by Abt's Institutional Review Board (IRB), and the study qualified for an exemption.

Data Analysis

Administrative Data

We used the following approach to handle the large volume of information available from the CCI documents. First, we applied a semi-automated data scraping procedure to retrieve the information that was standardized across the annual reports, such as participant names, partner organizations, and products developed. We used Python programs to parse the HTML versions of the annual reports to extract text included under standardized headers into an Excel spreadsheet. Annual reports prior to 2012 had a different structure and were saved as PDF files and converted to text strings. We identified relevant text based on standardized section headers. Given the nature of PDF format, text conversions were often imprecise and required manual review and correction. We also developed rules to align categories across reports, as they changed over the years. For example, in the old form, all senior staff were called Senior

[34] Interviews were spread over a long period of time due to a delay in clearance for data collection from the Office of Management and Budget (OMB). Pilot interviews with Co-Investigators; and interviews with NSF staff, Site Visitors, and non-CCI center PIs were conducted prior to OMB clearance, while interviews with the remaining respondents were conducted only after the receipt of OMB clearance.

Personnel, while in the new form they were further divided into PIs and Co-Investigators. All scraped data were manually reviewed, cleaned to remove duplicate data and convert all data to consistent categories, and summarized.

Second, we manually coded open-ended text from all available administrative records using a Microsoft Access database. To ensure consistency, senior staff piloted the coding scheme, which was based on the indicators developed during the design phase, on several representative documents. Based on this experience, we drafted a coding protocol that defined each indicator, provided specific examples for the type of information to code, and included guidance on which sections of the documents were most likely to contain these data. The protocol also identified indicators to be coded by two senior staff with doctorates in chemistry. The coding team, which contained nine researchers, was trained on the protocol in a two-hour session.

Coders were trained to review each document assigned to them, summarizing in the database all information relevant to each indicator that was included in the document, along with the document and page number where the information was found and any noteworthy quotes. Within each center, each type of activity (e.g., mentoring of graduate students by postdocs) or accomplishment (e.g., received a patent) described in annual reports, attachments, or proposals was coded as a separate instance. To capture external perspectives on the centers, coders reviewed site visit reports, oversight or funding memoranda, internal interim reviews, and review analyses; and documented both positive and negative assessments.

To ensure reliability of coding, all coders were assigned the same set of documents to code for one pilot center. Senior staff reviewed each coder’s work on the pilot center for consistency and completeness. All discrepancies were discussed and the coding instructions updated to further clarify any ambiguities that emerged during this pilot process.

Because the research accomplishments described in the administrative records were of a highly technical nature, two chemists coded this information for all centers and prepared profiles for each CCI summarizing all research accomplishments. These were submitted to NSF separately and are not included in this report. The remaining seven coders were assigned between one and three centers and asked to focus on non-technical information. The coding team met weekly to discuss progress and resolve questions on the coding procedures, indicator definitions, and how to handle specific challenging cases. Additionally, the database manager was on call during the coding process to resolve technical problems and track progress. After all center documents were coded, senior coders reviewed and cleaned the data to ensure consistency. The resulting data were summarized as the narrative included in this document.

Publication Data

We used comparative short interrupted time series (C-SITS) models to test whether trends in publications, citations, and co-authorship corresponded with Phase I and Phase II CCI award dates. The C-SITS models estimate a linear regression for each group (Phase I-only, Phase I/II, and Comparison) with discontinuities at the Phase I/Comparison award date and Phase II award date. We use a linear baseline trend model, as the bibliometric indicators appear to have time trends in the pre-award years. The models take the following form:

$$Y_{it} = \beta_0 + \alpha_{0i} + \beta_{1i}(year) + \sum_{p=1}^{9} \beta_{2p}(period * group)_p + \sum_{p=1}^{9} \beta_{3p}(period * group)_p * year + \varepsilon_{it}$$

where,

Y_{it}	=	the bibliometric outcome (publications, citations, or co-authorship) for the i^{th} investigator in the t^{th} time point.
β_0	=	the intercept, which is the overall mean for Phase I/II investigators in Year 0 (Phase I award year).
α_{0i}	=	is the deviation of investigator i's intercept from the mean intercept, distributed with mean 0 and variance σ_i^2.
β_{1i}	=	is the deviation of investigator i's slope, distributed with mean 0 and variance σ_{1i}^2.
β_{2p}	=	the intercept of each group in each period (e.g., Comparison in Period 0, Phase I/II in Period 2).
β_{3p}	=	the slope of each group in each period (e.g., Comparison in Period 0, Phase I/II in Period 2).
ε_{it}	=	the random error effect representing the difference between the value for investigator i in year t and the predicted mean value for the same group in year t. These residual effects are assumed normally distributed with mean 0 and variance σ_{it}^2, and are assumed to have 1^{st} order autoregressive correlation.

Because the model estimates random slopes and intercepts for each investigator and includes a first order autoregressive correlation, prediction lines may not track exactly with raw group means in each year. We have included the means on all bibliometric plots to illustrate show that a linear baseline trend model is a reasonable fit for the data. Since the most recent CCI Phase I awards included in this study were made in 2012, we restricted this analysis to five years before to six years after Phase I awards. To maintain a consistent sample for the entire analysis period, only CCI investigators who participated in the Phase I centers are included in the Phase II period (i.e., investigators who only joined the centers in Phase II were excluded). Additionally, investigators with a level of publications in the top one percentile of the sample (more than 93 in a year) were excluded from the primary analysis, given the high probability that their data combined publications from multiple individuals with the same name. Sensitivity analyses for the full sample are presented in Appendix F.

We also generated chord diagrams to illustrate patterns of co-authorship within Phase I/II centers by creating a matrix of all possible pairs of investigators within a center that contained the number of papers each pair co-authored. We used Python to create chord diagrams for each center.[35]

Surveys

We used descriptive statistics to summarize survey data. These included calculating frequency distributions and percentages to summarize measures on categorical scales, and cross-tabulations to illustrate differences in measures between groups or the distribution of measures across subgroups of interest.

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35 The Python script to create the chord diagrams is archived on a public GitHub site (https://github.com/NETESOLUTIONS/ERNIE/blob/master/Scopus/Abt_Analysis/Analysis_scripts/chord.py).

Since survey response rates were less than 80 percent, we performed two sets of analyses to assess the implications of non-response. First, characteristics of individuals who completed the surveys were compared to those who did not, although the number of individual characteristics available from annual reports was very limited. We compared PIs/Co-Investigators on center affiliation and whether they were affiliated with the CCI lead institution, and we compared graduate students/postdocs on center affiliation and their most senior project role (graduate student or postdoctoral scholar). Second, we calculated the probability that a participant in each category (Center*Lead Institution for PIs/Co-Investigators, Center*Role for graduate students/postdocs) was located and responded to the survey request. To account for non-response bias, inverse probability weights were created based on the salient baseline characteristics and used in frequency calculations.[36] Weights for the PI/Co-Investigator survey ranged from 1 to 4 (mean 1.5), and weights for the Graduate Student/Postdoc survey ranged from 1.5 to 3.5 (mean 2.3). To test for significant differences in proportions by subgroup, we used a difference in means test with variance estimated using the delete-1 jackknife method.

Interviews

Qualitative responses from interviews were synthesized, cleaned, and standardized before being uploaded into *NVivo*, a qualitative data analysis software package. We developed preliminary sets of themes based on interview questions. An inductive coding process was used, so that themes were refined or new themes were generated in response to emergent topics within the responses. Data were summarized by stakeholder groups and compared across groups. The themes that emerged are presented in this report and illustrated with quotes. Every effort was made to protect respondent identity and to avoid comparing the centers to each other.

Evaluation Schedule and Changes to Original Scope

The evaluation occurred in three phases: (1) evaluation design and planning, (2) data collection and analysis, and (3) reporting. The original schedule was delayed due to the government shutdown in January 2019 and a delay in the receipt of OMB clearance. The final schedule for each phase of the study is specified below:

• **Phase 1 – Evaluation Design and Planning**	**October 2017–April 2018**
• **Phase 2 – Data Collection and Analysis**	**May 2018–August 2019**
- Preparation of OMB clearance package	May–September 2018
- Receipt of OMB clearance	May 2019
- Administrative data collection	August–October 2018
- Administrative data analysis	November 2018–March 2019
- Bibliometric data collection and analysis	December 2018–August 2019
- Survey data collection	May–July 2019
- Survey analysis	July–August 2019
- Interview data collection	May 2018–August 2019
- Interview data analysis	January 2019–August 2019

36 For example, assume that 5 of the 10 PIs/Co-Investigators at non-lead institutions in a particular center completed the survey. The respondents would receive inverse probability weights of 2 (10/5). Each respondent's answers would be weighted to account for one of their non-responding colleagues.

- **Phase 3 – Evaluation Reporting** **September–December 2019**
  - Draft Evaluation Report September–October 2019
  - Final Evaluation Report October–December 2019

Over the course of the study, several changes were made to the original study design:

- **Research Questions** – We made minor changes to the wording of five of the original questions (RQ 1, 1.1, 1.4, 2.1, and 4.1) to ensure they could be feasibly answered using the proposed design and available data. For example, we removed the term "impact" from two of the research questions. While we are aware that this term is often used in federal evaluation contexts, it is more accurate to apply it to quasi-experimental or experimental designs, which are not feasible for this study. We also removed the wording "to what extent" in instances when we think reliable quantification would not be possible.
- **Interview Sample** – We reduced the number of Co-Investigators interviewed, since they were providing similar information to the PIs and were also asked to complete a survey. In addition, we included Managing Directors who early on emerged as key to center operation and activities. Finally, we interviewed Site Visitors and Industry Partners to obtain an external perspective on the centers.
- **Publication Extraction Method and Sources –** To construct a dataset of CCI-acknowledging papers, we initially attempted to query Scopus for items listed in annual reports, but found that many of these did not yield any hits (presumably because they were either never published or published under a different title). Instead, we used CCI grant numbers to query both Scopus and Web of Science.
- **Creating Profiles for each Phase II CCI –** Using data from annual reports and renewal proposals, we developed a profile for each Phase II center that included a brief description of its mission and the list of scientific advances culled from these documents. While our team include PhD-level chemists and biologists, we were unable to judge the importance of these discoveries. The profiles were submitted to NSF and can be used as a source of data for an expert panel.

Study Oversight

We took advantage of two evaluation oversight strategies proposed by NSF. First, throughout the study we regularly met with the NSF evaluation team and CCI Program staff to discuss the program, data sources, data collection and analysis strategies, comparison groups, challenges, and reporting preferences. We also submitted to NSF interim memoranda describing our findings from administrative data, the bibliometric analysis, and survey/interview data, and received feedback on their clarity and content. Finally, we presented the findings available to date at two in-person meetings with NSF staff.

Second, with input from NSF, we selected and convened a distinguished, external seven-member Technical Working Group (TWG) of experts in chemistry, research program evaluation, bibliometrics, and Science, Technology, Engineering, and Math (STEM) policy. The following individuals served on the TWG:

- Prof. Victor Batista, Yale University (chemistry)
- Dr. Emilio Bunel, Director of Division of Chemical Sciences and Engineering, Argonne National Laboratory (chemistry)
- Prof. Melissa Hines, Cornell University (chemistry)

- Prof. Tara Meyer, University of Pittsburgh (chemistry)
- Dr. Kevin Boyack, President, SciTech Strategies (bibliometrics)
- Dr. Daryl Chubin, independent consultant (STEM policy and program evaluation)
- Dr. Gretchen Jordan, independent consultant (innovation and program evaluation).

TWG members contributed both to the study design and the interpretation of findings by reviewing the evaluation plan and the draft report, and by participating in two teleconferences to discuss these documents, at the beginning and end of the study. We used the feedback offered at the first session to adjust our evaluation approach by increasing our reliance on the external perspective about the program by conducting interviews with CCI Site Visitors and reviewing relevant administrative records. We used the feedback offered at the second session to adjust our conclusions and recommendations.

Study Limitations

The data collection approaches used for this study have several limitations, which may affect the validity of the data and/or their interpretation.

General Limitations and Challenges

First, we cannot definitively attribute changes in CCI outcomes and outputs to program participation. This type of design requires random assignment or some other comparison group and is not practical for the CCI Program. While we did include a comparison group in the publication analysis, we did not have the data to control for potentially important confounders, such as participation in non-NSF centers by PIs in our “individual investigator” group. We also interviewed PIs of non-CCI centers to understand differences in perspectives of PIs in other center programs, but non-CCI centers that we included as a comparison were quite different from CCIs, and the number of individuals in the groups were too small to go beyond anecdotal comparisons.

The second general limitation was the timeframe of the study. The earliest Phase II centers had only recently completed their full term, making it difficult to capture important contributions to the field or societal outcomes. Given that the CCI Program focuses on making advances in fundamental chemistry, the gap between the research and these types of outcomes could be particularly long.

Third, we could not fully answer some NSF questions or collect data on all indicators. For example, we were unable to operationalize and systematically measure “leadership” in the context of both research and non-research activities of CCIs, and the indicators of benefits to society were limited to commercialization and workforce development. Furthermore, we could not fully answer the research question about the contribution of CCIs to fundamental chemistry. While we painstakingly compiled the data on accomplishments for each Phase II center, we did not have the expertise to judge their importance or influence. This task is performed by an expert panel in the future.[37]

Fourth, we were limited to self-reported data, primarily from CCI participants, in measuring how the chemistry research community benefited from the CCI centers and whether and how CCIs contributed to institutional change.

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[37] We discussed convening such a panel for this study with NSF, but ultimately decided against it, in part due to lack of time.

Finally, NSF requested that we organize the study findings by sub-question, which we found challenging as some of the data responded to multiple questions. For example, sub-question 1.3, which asks whether the center mechanism of operation contributes to the research achievements of the center, considerably overlaps with RQ 4, which is about the effectiveness of the center's structures and operations in achieving the program's goals. We did our best to adhere to the question-based layout, while trying to avoid duplicating the information or disrupting the narrative flow.

Administrative Data

The primary limitation of these data was the consistency and completeness of the documents, which varied from center to center and year to year. While reviewing administrative records for the same center, coders attempted to combine instances that clearly represented the same activity and listed all data sources where this information could be found. However, in many cases, it was impossible to determine with certainty whether a given instance represented the same or a new activity (e.g., a vaguely described seminar series, tool, or after-school program). Another challenge was that many activities were relevant to multiple indicators. To avoid generating highly duplicative information, coders were instructed to code activities to the most relevant indicator, rather than to all applicable indicators. For these two reasons, we did not count instances of each activity or accomplishment, but instead focused on capturing their types. Finally, we were unable to discern patterns of improvement over time from an external perspective, as oversight personnel did not necessarily discuss the same issues across years and tended to include both positive and constructive feedback in each report.

Publication Data

One of the well-known challenges of publication analysis is a contamination of data by unrelated individuals with the same names. To the extent possible, to resolve these cases, we tried to limit author profiles using disciplinary filters. Other problems for these data included having multiple persons with the same Author ID or multiple Author IDs for the same person, duplicate profiles, and changes in names or affiliation. As mentioned above, we also experienced challenges identifying publications attributable to CCI funding. Extensive testing and manual curation were necessary to create the publication datasets.

Surveys and Interviews

Survey and interview data are self-reported and prone to "social desirability bias" (i.e., respondents may exaggerate their accomplishments and minimize challenges because they think this is what the funder or evaluator wants to hear). Careful formulation of the questions, asking similar questions in a different way, probing, assurances of confidentiality, and collection of similar data from multiple groups of respondents partially mitigates this problem.

Another limitation is the potential for recall bias, which can occur when events being asked about happened in the distant past. To minimize this bias, we limited the sample to the PIs/Co-Investigators who participated in the program no earlier than the 2012–2013 reporting year and graduate students/postdocs who participated no earlier than the 2014–2015 reporting year (approximately six years or less before data collection). In addition, as mentioned above, survey questions asking for information that might be difficult to recall included options such as "do not recall or uncertain," screening out individuals who could not recall being part of the centers.

Due to the limited period of time available for data collection and the suboptimal timing of survey administration resulting from the OMB delay and the government shutdown, response rates were not as high as initially anticipated. It is thought that data collected from less than 80 percent of study subjects may not represent the views of the entire population, as respondents with extreme positive views may be more likely to complete the survey, while individuals with negative views may wish to avoid responding. We attempted to address this limitation by adjusting the data for non-response, as described above. However, the set of available individual characteristics was limited (center, lead/non-lead institution, and role in CCI), and it is likely that important differences between respondents and non-respondents were not captured.

Finally, the interview samples with the exception of PIs and Managing Directors included a small subset of respondents who may not be representative of their populations. Furthermore, we excluded some potentially identifiable information gathered in interviews to protect the anonymity of respondents, many of whom are well-known to NSF.

We note that most of these limitations (e.g., lack of comparison groups, self-report, recall bias, low response rates) are common to all evaluations of research programs.

Chapter 3: Research Question 1 Findings

Data reported in Chapters 3–7

In these chapters, we address RQs and sub-questions posed by NSF for the study. Each chapter draws on all quantitative and qualitative data available from four data collection modalities. In the narrative, we identify each source and indicate any discrepancies between sources. In the beginning of each chapter, we include a table that shows to what extent we were able to answer each sub-question, accompanied by brief explanations. Finally, the exhibits displaying survey data generally include a subset of responses to highlight particular findings. We include tables with all responses to survey items in Appendices H and I, and tables with the data used to create each chapter exhibit in Appendix J.

RQ 1: What are the important contributions of the CCI Program to our current understanding of fundamental chemistry?

Sub-Question	Extent Addressed	Comment
1.1 What is the evidence of productivity and influence of the scientific research?	●	Fully addressed in this chapter.
1.2 To what extent and in what ways have the CCI centers demonstrated both leadership in their field and responsiveness to developments in their field?	◕	Leadership not consistently defined. Responsiveness addressed in RQ 1.4 and RQ 4.
1.3 Does the center mechanism of operation contribute to the research achievements of the centers?	●	Addressed in RQ 4.
1.4 In what ways has the chemistry research community benefited from the CCI centers?	◐	Limited to self-reported and anecdotal evidence.

Sub-question 1.1. What is the evidence of productivity and influence of the scientific research?

The study team reviewed annual reports and renewal proposals of the Phase II centers to identify all discoveries described. This effort yielded dozens of items per center, but we could not judge their relative importance because of the highly technical nature of the material. All accomplishments were documented in brief profiles that were prepared for each center and submitted to NSF.

CCI participation likely increased investigators' publication productivity and the contributions of their research to the scientific community

Another way to characterize scientific contributions is through bibliometric analysis. To examine the effect of CCI participation on research productivity, we analyzed publication records of the subset of 200 CCI investigators who participated in a Phase I center[38] over three time periods: (1) five years prior to Phase I, (2) during the three years of Phase I, and (3) six years after Phase I (the first three years of Phase II for awarded centers). As a comparison, we used a subset of 370 investigators on individual NSF

[38] We excluded 126 CCI investigators who joined a center in Phase II to keep a consistent sample throughout the analysis period.

grants in chemistry with award years aligned to the Phase I CCIs.[39] For each investigator, we examined the number of papers they authored in a particular year and the number of times a publication from a particular year was cited. All publications in both groups are included in this analysis, regardless of whether or not they acknowledged the CCI or the comparison NSF award.[40] Differences between groups may be confounded by unobserved factors (e.g., total amount of research funding) and should not be interpreted as causal impacts of CCI.

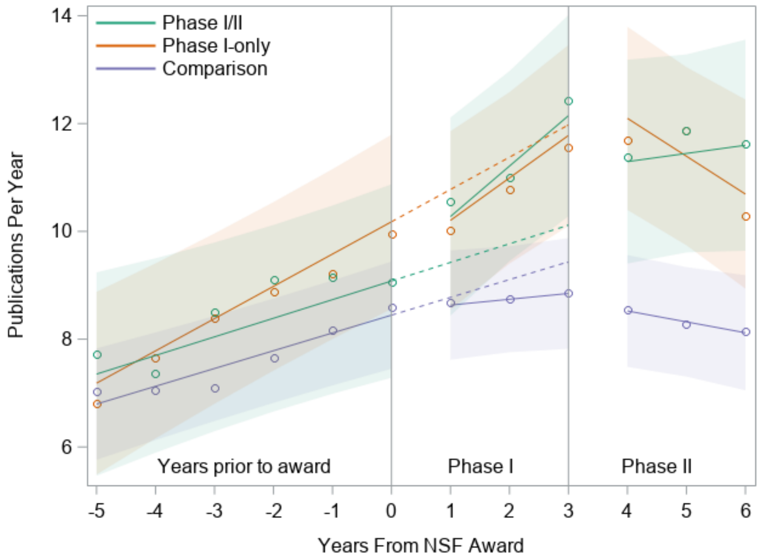
We found that in the period preceding the Phase I or comparison awards, all three groups exhibited similar productivity of approximately seven papers a year per investigator, on average (Exhibit 7). Publication volume increased gradually to 8 to 10 papers by the first year of Phase I or a corresponding comparison year. Up to that point, the trends between the groups were very similar, although the comparison investigators tended to have slightly lower productivity (the differences were not significant).

After the start of the Phase I or comparison award, productivity trends began to diverge. For all CCI participants, the number of publications increased over the three-year period from 10 to 12 per year per investigator. In contrast, the comparison investigators appeared to have lost momentum, producing about eight publications annually; the differences between CCI and non-CCI investigators were statistically significant ($p < 0.01$). Furthermore, publication patterns of the Phase I-only and of comparison investigators followed a fairly consistent gradual upward trajectory from year -5 to year 3. In contrast, the productivity gain among investigators with a Phase II award exceeded the trend established in the pre-award period during the Phase I award ($p < 0.01$) and outpaced the other two groups. The trends in the next three-year period were also interesting. Investigators in the Phase II group continued publishing at approximately the same rate of around 12 papers per year, but investigators in Phase I-only and in comparison groups showed a decline to 11 and 7 papers, respectively.

39 We excluded 127 comparison investigators with awards after 2012 to keep a consistent sample throughout the analysis period.

40 Investigators with number of publications in the top one percentile of the sample (more than 93 in a year) were excluded from the investigator-level bibliometric analysis, given the high probability that their data inadvertently combines publications from multiple individuals with the same name. Sensitivity analyses with the full sample (including the top percentile) are presented in Appendix F.

Exhibit 7: Phase II Investigators Exceeded Pre-Award Trends in Publications during Phase I and Maintained High Productivity Levels in Phase II



Notes: Phase I/II investigators (N = 86, excluded = 2), Phase I-only investigators (N = 114, excluded = 3), comparison investigators (N = 370, excluded = 10), and investigators in the top one percentile of publications are excluded from the model. Hollow circles represent average values by group (average number of publications per investigator in a particular year). Solid lines represent linear-predicted values, separated by period. Estimated models are interrupted time series, so discontinuities occur at each period boundary. Colored bands represent 95% confidence intervals around predicted values. Overlapping confidence intervals signify that predicted values do not significantly differ between groups. Dashed lines represent extrapolations of the pre-award period trend into the Phase I period. Prediction models include random slopes and intercepts at the individual level and a first-order autoregressive structure.

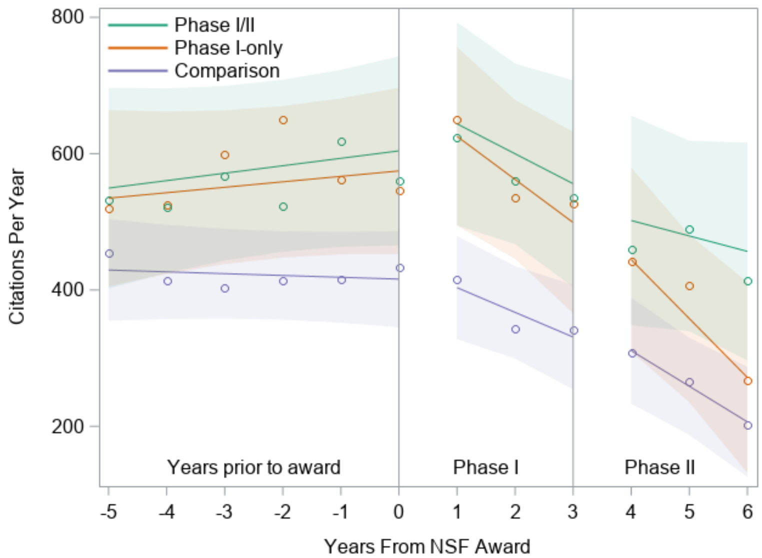
Source: all publications in Scopus authored by CCI investigators who participated in Phase I and comparison investigators.

We also examined the impact of publications on the research community by measuring citation counts[41] for the three groups of investigators over the same three time periods. Both Phase I-only and Phase I/II investigators were more highly cited before the CCI award than the comparison group, at approximately 600 citations per year per CCI investigator versus approximately 400 for a comparison investigator ($p < 0.05$; Exhibit 8). This trend continued after the CCI award. For all three groups, citations decreased over time at a similar rate. Publications in later years had less time to accumulate citations, most likely explaining the downward trend, but other reasons are also possible.

In addition to analyzing the entire publication output for CCI and comparison investigators, we examined the trends for a set of 2,054 publications that acknowledged a CCI grant (hereafter referred to as CCI-acknowledging publications). These are on a per-center rather than per-investigator level to avoid double-counting publications of co-authors. We found that by the end of CCI year 3, Phase I-only and Phase I/II centers published at similar levels of six and eight papers per center annually. In contrast, three years after the end of the Phase I award (year 6), the average number of CCI-acknowledging papers increased to 26 per center for the Phase I/II centers, while declining to 0 for the centers that did not participate in Phase II (e.g., received no CCI funding past year 3; $p < 0.001$; Exhibit 9).

41 Citation counts include self-citations.

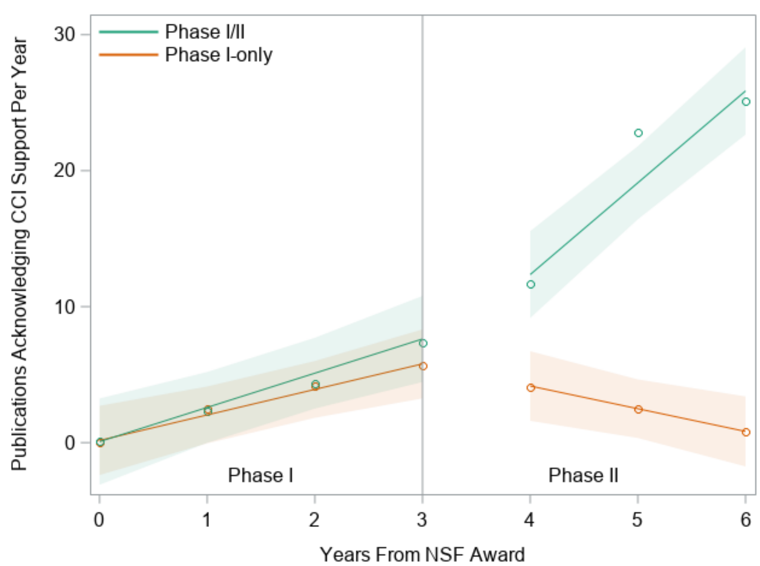
Exhibit 8: CCI Investigators Are More Highly Cited than Comparison Investigators



Notes: Phase I/II investigators (N = 86, excluded = 2), Phase I-only investigators (N = 114, excluded = 3), comparison investigators (N = 370, excluded = 10), and investigators in the top one percentile of publications are excluded from the model. Hollow circles represent average values by group (average number of citations of an investigator's publications from a particular year including self-citations). Solid lines represent linear-predicted values, separated by period. Estimated models are interrupted time series, so discontinuities occur at each period boundary. Colored bands represent 95% confidence intervals around predicted values. Overlapping confidence intervals signify that predicted values do not significantly differ between groups. Prediction models include random slopes and intercepts at the individual level and a first-order autoregressive structure.

Source: all publications in Scopus authored by CCI investigators who participated in Phase I and comparison investigators.

Exhibit 9: Phase II Award Increased Center-Level Publication Productivity

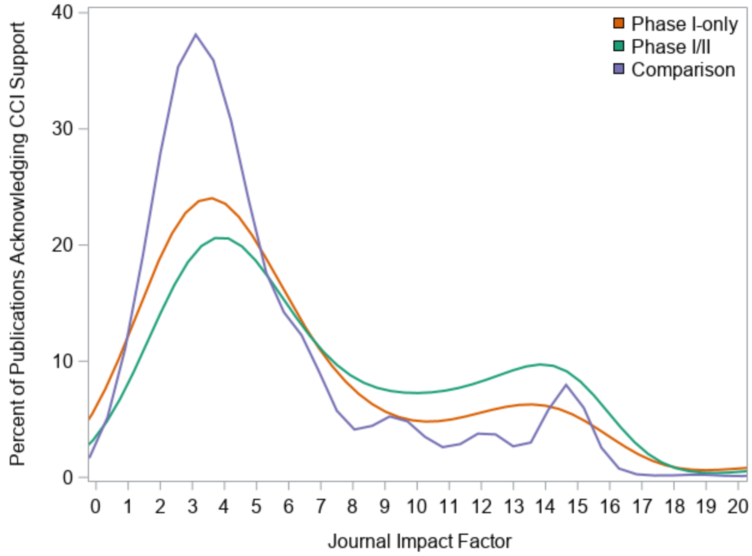


Notes: Phase I/II centers (N = 9) and Phase I-only centers (N = 14). Hollow circles represent average values by group (average number of publications that acknowledge a center in a particular year). Solid lines represent linear predicted values, separated by period. Estimated models are interrupted time series, so discontinuities occur at each period boundary. Colored bands represent 95% confidence intervals around predicted values. Overlapping confidence intervals signify that predicted values do not significantly differ between groups. Prediction models include random slopes and intercepts at the center level and a first-order autoregressive structure.

Source: all publications in Scopus and Web of Science that acknowledge CCI support.

Finally, we analyzed the distribution of journal impact factors (a measure of journal quality)[42] for CCI-acknowledging publications and for a random sample of publications by comparison investigators. The calculations revealed that Phase I/II centers published papers in journals with significantly higher-impact factors than Phase I-only centers, with an average impact factor of 9.1 versus 7.9 ($p < 0.05$; Exhibit 10). Furthermore, CCI-acknowledging publications for both phases appeared in journals with significantly higher impact factors than the average for publications from a random sample of comparison investigators, which was 6.1 ($p < 0.001$; Exhibit 10).

Exhibit 10: CCI-Acknowledging Publications had Higher Impact Factors than Typical for the Field and Phase I/II Outperformed Phase I-Only Centers



Notes: Curves represent nonparametric kernel density estimates using normal weight functions.

Source: all publications in Scopus and Web of Science that acknowledge CCI support (N=2,054). Journal impact factors were obtained from the JCR 2018 dataset. The comparison sample includes 2,000 publications with journal impact factors. 191 publications (19 Phase I-only, 113 Phase I/II, and 59 Comparison) with journal impact factors above 20 are not shown.

Productivity data collected in the online survey were consistent with bibliometric indicators: since joining the centers, 65 percent of CCI PIs and Co-Investigators reported publishing more papers, 43 percent publishing in higher-quality journals, and 45 percent in a broader range of journals (Exhibit 11).

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42 Journal impact factor is the average number of citations per article in a journal per year.

Exhibit 11: CCI PIs and Co-Investigators Reported Increased Productivity, Diversity of Publications, and Journal Quality

Notes: N = 134, Missing = 5–8.

Source: Survey of Principal Investigators and Co-Investigators Q9 (Have any of the following changes occurred in your publication patterns, research interests, and/or professional visibility since you began participating in CCI?).

Sub-question 1.2. To what extent and in what ways have the CCI centers demonstrated both leadership in their field and responsiveness to developments in their field?

We found that the concept of leadership in research is difficult to define and measure. The literature review performed during the initiation phase of the evaluation yielded limited data on this topic (Appendix A). Perhaps not surprisingly, when asked about leadership in interviews, respondents were either unable to answer the question or offered a broad range of examples. Site Visitors, NSF staff, and CCI PIs said that center participants are well-known scientists who work on difficult and important scientific challenges, and use new instrumentation and methods. High-profile CCI publications (including the best paper in *Science*), large professional networks, leveraged funding, invitations to important conferences, and relevance to industry were also cited as evidence of leadership. For example, one Co-Investigator said that their center aims to "shape the narrative of the field" by organizing conferences, writing "for the right journals," and generally being visible to the community. A Managing Director reported that 100 of their alumni had faculty positions at top institutions in the United States and worldwide, and that they had started two journals, of which one has one of the highest impact factors. NSF staff and a Site Visitor indicated that many scientists want to join the centers, and another Site Visitor said that a publication from one CCI led to important work in his group. Finally, two Co-Investigators highlighted the leadership role CCIs play in mentoring junior scientists and collaborating with minority-serving institutions. One of the two said that participating in CCI helped him build a professional network that would otherwise have taken decades to establish. We collected extensive evidence such as these from other sources.

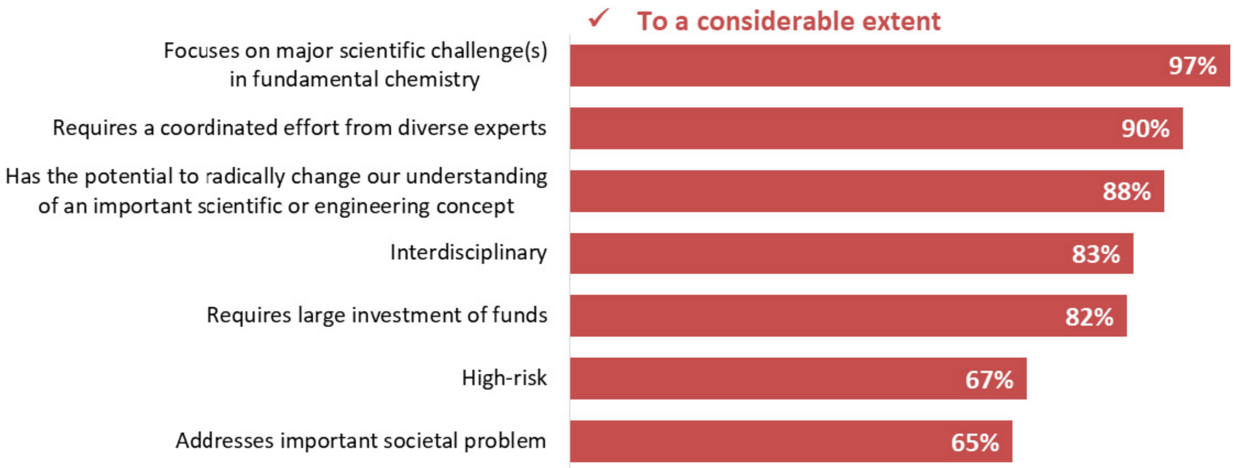
> *"A number of the people involved [in CCI] that weren't household names amongst chemists now are. But just seeing the publication outcome, I think is really excellent. So in this particular one [CCI], I think the money was well spent."*
>
> *"I got inspiration from a paper that I saw coming from [CCI participant names redacted]. It has now led to one of the major projects in my group."*
>
> *–Site Visitors*

CCIs focus on difficult and important scientific challenges

One way to demonstrate leadership is to tackle important societal problems that have been resistant to solutions because they are too risky, require interdisciplinary approaches, necessitate costly equipment, or for some other reason. This construct of leadership is at the heart of the CCI Program, which is based on the idea that bringing together teams of scientists and offering them generous and long-term support may "move the needle" on unsolved fundamental problems. We designed a survey item to examine the work of CCIs in that context.

The majority of investigators indicated that their research addressed a major challenge in chemistry and an important societal problem (97 percent and 65 percent, respectively), had the potential to radically change our understanding of an important scientific or engineering concept (88 percent), and was interdisciplinary and high-risk (83 percent and 67 percent, Exhibit 12). Virtually all respondents also reported that their research required a coordinated efforts of diverse experts and large investment of funds (90 percent and 82 percent).

Exhibit 12: CCIs Show Leadership by Focusing on Major Scientific Challenges that Require a Large Investment of Funds and Have the Potential to Radically Advance the Field



Notes: N = 134, Missing = 0–1.

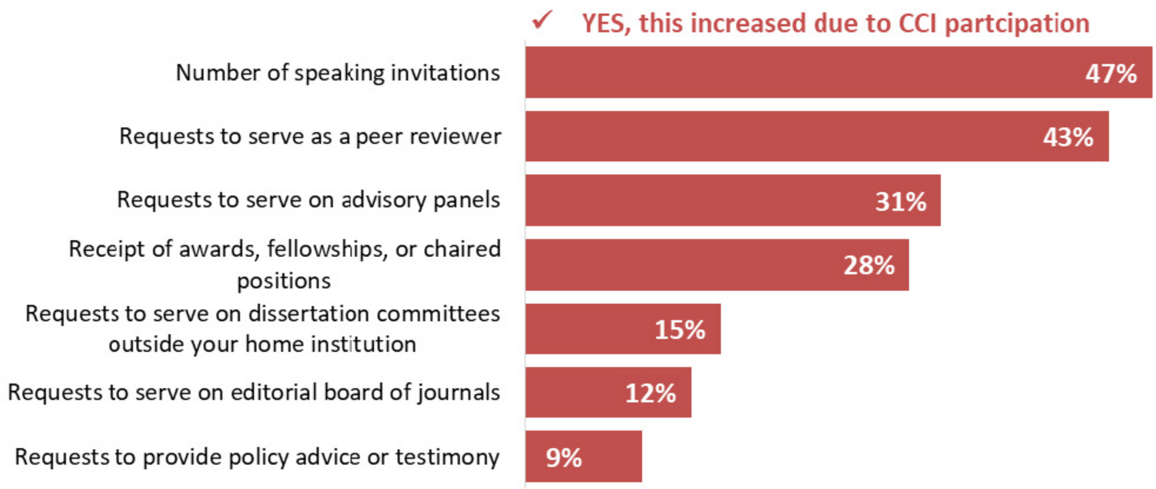
Source: Survey of Principal Investigators and Co-Investigators Q4 (To what extent does the research conducted by your CCI have the following characteristics?).

CCI funded well-known scientists whose standing was further enhanced through participation in the program

Administrative records provided extensive evidence that CCI researchers are well-respected members of the chemistry community. Several centers reported that their participants served as advisors, editors, and panelists, suggesting that their judgment is valued (one center listed 42 external organizations for which its participants play these roles). In addition, center reports mentioned numerous awards, prizes, and other honors received by their faculty. Particularly notable of these were the MacArthur Fellowships, awarded to faculty at two different centers, an induction into the National Academy of Sciences, and an invention selected as one of the 50 Best Inventions of the year by *Time Magazine*.

In the survey, PIs and Co-Investigators made a direct connection between CCI participation and improved professional outcomes. After joining the center, survey respondents received additional invitations to present at conferences (47 percent); serve on advisory panels (31 percent), peer-review committees (43 percent), editorial boards of journals (12 percent), and thesis committees (15 percent); and provide policy advice or testimony (9 percent; Exhibit 13). More than a quarter also reported new awards, fellowships, and other honors such as endowed chairs.

Exhibit 13: CCI PIs and Co-Investigators Reported Improved Professional Outcomes



Notes: N = 134, Missing = 5–8.

Source: Survey of Principal Investigators and Co-Investigators Q9 (Have any of the following changes occurred in your publication patterns, research interests, and/or professional visibility since you began participating in CCI?).

Similar data on the benefits of CCI participation were obtained in interviews. CCI PIs and Co-Investigators credited the program with expanding their professional networks; helping them publish higher impact, more visible papers; developing their leadership skills; and giving them the opportunity to work on problems of real-life importance. One CCI PI said that he became famous because of the outreach program launched by the center, and another was elected to the National Academy of Engineering because of CCI research. Interviewees cited many specific scientific contributions of their centers, which they said would not have been possible to achieve without CCI.

Sub-question 1.3. Does the center mechanism of operation contribute to the research achievements of the centers?

This question is addressed under RQ 4.

Sub-question 1.4. In what ways has the chemistry research community benefited from the CCI centers?

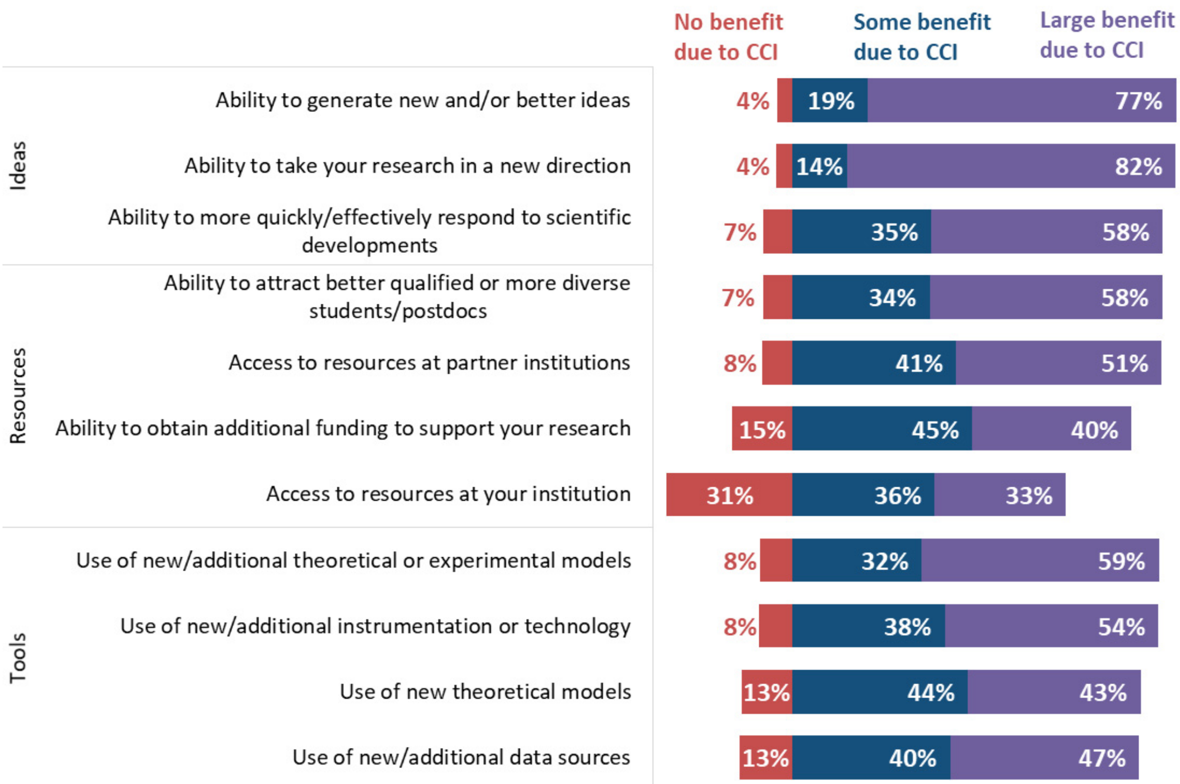
CCI participants derived many benefits from the centers

Survey respondents indicated that participating in the CCI Program offered many benefits. Being part of the center helped them recruit better students and postdocs (92 percent); obtain additional funding (85 percent); access resources at their own or partner institution (69 percent and 92 percent, respectively); and apply new theoretical models, data sources, and instrumentation/technology (87 percent, 87 percent, and 92 percent, respectively; Exhibit 14). Survey respondents also said that CCI participation enabled them to work on more diverse problems (75 percent, data not shown),[43] generate better ideas (96 percent), take work in a new direction (96 percent), and more quickly/effectively respond to scientific developments (93 percent). Further analysis of survey data revealed that access to resources may differ for various partners in a center. Researchers at lead institutions were more likely to say that they benefited

[43] Appendix H, Exhibit H-6, presents complete information for this survey item.

from resources available at their own organization (90 percent versus 55 percent, $p < 0.001$, data not shown), while researchers at non-lead institution were more likely to say they benefited from resources at partner organizations (99 percent versus 83 percent, $p < 0.05$, data not shown).[44]

Exhibit 14: CCI Helped Investigators Generate New Ideas and Broaden their Research Program



Notes: N = 134, Missing = 0–1, Not applicable = 4–14.

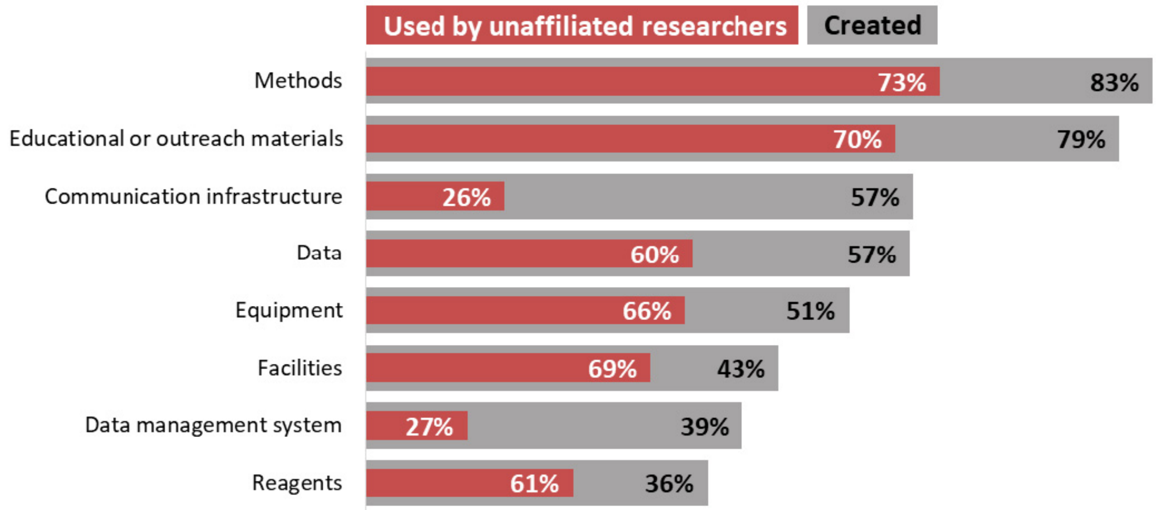
Source: Survey of Principal Investigators and Co-Investigators Q8 (Please indicate whether participation in the CCI has benefited your research program).

CCI resources were used by the broader community

In the survey, we also asked CCI PIs and Co-Investigators whether they developed various resources and if these resources are used by researchers outside of the centers. The most frequently reported were methods and educational/outreach materials (approximately 80 percent); followed by communication infrastructure, data, and equipment (approximately 50–60 percent); and reagents, data management systems, and facilities (approximately 40 percent; Exhibit 15). Among the resources developed, methods, data, equipment, facilities, and reagents appeared to be particularly widely used by researchers not affiliated with CCIs; while communication infrastructure and data management systems were not. This is not surprising, as these latter resources were created primarily to support the centers.

[44] Appendix H, Exhibit H-5, presents complete information for this survey item.

Exhibit 15: Various Resources Created by CCIs are Being Used by Researchers Outside of the Center



Notes: Q10 N = 134, Missing = 0. Q10A N = 111, Missing = 0.

Sources: Survey of Principal Investigators and Co-Investigators Q10 (Which of the following resources have been created or improved by CCI?); Q10A (Which of these resources, if any, are being used by researchers not affiliated with the center?).

Responses for Q10 may not sum to 100% because multiple responses were permitted. Responses for Q10A are limited to respondents who indicated the resource was created or improved by CCI in Q10. Inner bar values are expressed as a percentage of the corresponding outer bar.

Additional information about resources generated through the program was available from administrative records. Some centers described costly equipment, facilities, technologies, and tools acquired with grant funding, such as an electron microscope, an aerosol spray research facility, and a fabrication laboratory to build novel instrumentation. Other centers mentioned innovations such as microplasma arrays, hydroxy acid mediated peptide synthesis, nonenzymatic DNA ligation, and solution-deposited inorganic photoresists. Yet others reported new computational tools to design, predict, and identify molecules; and to process large datasets generated through experiments.

> *"What the CCIs have done is really enabled and enforced collaboration in a way that has been really good for the field."*
>
> *–Site Visitor*

Finally, we discussed the broader use of CCI resources in key informant interviews. Industry Partners indicated that CCI ideas led to new technologies developed by their companies and that their technologies were tested by CCIs. These partners also highlighted the advantage of CCIs in bringing so much expertise to bear on a problem. Finally, CCI internship programs helped the companies recruit talented young scientists. The contributions of CCIs to the scientific community mentioned by Site Visitors and NSF staff included scientific discoveries, successful models for interdisciplinary collaboration, new instruments, and a highly qualified workforce. These respondents also argued that high-profile results from CCIs have reached the general public, making a strong case to taxpayers of the benefits of basic research.

Chapter 4: Research Question 2 Findings

RQ 2: How successful have the CCI centers been at transferring their basic research results into societal or economic benefits (innovation)?

Sub-Question	Extent Addressed	Comment
2.1 In what ways have the research findings and other center achievements contributed to societal and economic benefits?	◐	Lack of established definition for societal and economic benefits
2.2 In what ways have the CCIs developed partnerships to engage in technology transfer, to commercialize technology, or for other societal benefit?	●	Fully addressed in this chapter

Sub-question 2.1. In what ways have the research findings and other center achievements contributed to societal and economic benefits?

CCIs are translating research findings into commercial products

The review of the literature performed during the design phase of the evaluation revealed that societal and economic benefits of research are typically measured through commercial indicators, such as invention disclosures, licenses, patents, start-up companies, and manufactured products. Thus, we also focused on these outputs in this study.

Using two sources of patent data, we were able to verify 28 patents reported by CCIs (Appendix C). Of these, 75 percent acknowledged NSF, 68 percent the CHE, and 57 percent CCI funding. In addition to patents, most centers reported inventions, ranging in number from one to four per CCI, and a few reported licenses. Examples of CCI research commercialization described in annual reports included experimental methods (e.g., recovery of phosphorus from the atmosphere using ultraviolet light, hydroxy acid mediated peptide synthesis), devices/technologies (e.g., novel plasma ion source for mass spectrometry, novel high-yield metal-insulator-metal tunneling diodes), and new compounds and materials (e.g., new non-natural nucleosides, light absorbers, catalysts). To facilitate knowledge transfer to industry, one CCI planned to openly share all its innovations from NSF-funded work following a patent application. Some CCIs entered into licensing agreements with industries, which include Inpria, Hewlett Packard, IBM, and Intel. Finally, seven CCIs mentioned launching start-ups and one mentioned creating a spin-off company. The products being developed by these companies included plastics that are more degradable in solution, instrumentation to assess atmospheric aerosols in controlled laboratory settings, devices to store energy from renewable sources, and a polymer development platform for inhibition of RNA using therapeutic compounds.

> *"The innovation impacts thus far by the center are laudable. The demonstrated capabilities of the microscopy tools developed thus far have broad implications for the chemistry community."*
>
> *-Site Visit Report*

Non-center-generated administrative records and renewal proposals for almost all CCIs highlighted commercialization activities. For example, one center described having launched several companies and incorporated entrepreneurship as an educational component. A site visit report for another center described a culture of innovation, where students and postdocs are encouraged to learn the "language of business" and to think about how their research might be translated into products. However, the report also cautioned the center that students should hone their scientific skills before focusing too much on commercialization. Finally, other site visit reports indicated that new or improved instruments and other tools developed by CCIs would benefit many scientists, regardless of the field.

Sub-question 2.2. In what ways have the CCIs developed partnerships to engage in technology transfer, to commercialize technology, or for other societal benefit?

CCIs developed ties to many partners and benefited from these relationships

Data included in annual reports indicated that all CCIs partnered with a range of organizations in both funding phases. The average number of partners per CCI for the nine Phase I/II centers doubled from 12 to 24 between the first and second phases (Exhibit 16). Each center had at least one partner, with one CCI reporting 43 partners.

We also examined the types of organizations that partnered with CCIs. U.S. academic institutions and industries appeared the most common, reported by six–nine CCIs in each phase (Exhibit 16). Smaller numbers of centers also partnered with foreign academic institutions, nonprofits, national laboratories, federal agencies, schools, and professional associations.

Exhibit 16: Phase I/II CCIs Partnered with a Broad Range of Organizations

Partner Contribution	Phase I Award				Phase II Awards			
	# Centers with Type of Partner	# Partners per Center			# Centers with Type of Partner	# Partners per Center		
		Average	Min	Max		Average	Min	Max
Any partners	9	12	1	43	9	24	4	43
U.S. academic institution	6	5	1	9	9	10	1	17
Industrial or commercial firms	7	9	1	31	8	9	1	19
Foreign academic institution	2	4	3	4	6	2	1	4
Other nonprofits	3	1	1	2	6	2	1	4
National laboratory	2	1	1	1	3	2	1	3
Federal agency	0	0	0	0	2	2	1	3
School or school systems	2	4	2	5	1	1	1	1
Professional association	1	1	1	1	1	1	1	1

Sources: Phase I and Phase II Annual Reports from Phase I/II CCIs between 2004 and 2016 – Participants/Organizations.

In annual reports, CCIs also described the nature of these partnerships. The most frequently mentioned was engagement in collaborative research, reported by seven Phase I and nine Phase II centers (Exhibit 17). This was followed by the use of facilities, support for K-12 programs, financial contribution, in-kind contribution, and support for student career development.

Exhibit 17: Phase I/II CCI Partnerships included Various Types of Relationships

Partner Contribution	Phase I Award				Phase II Awards			
	# Centers with Type of Partner	# Partners per Center			# Centers with Type of Partner	# Partners per Center		
		Average	Min	Max		Average	Min	Max
Advisory board/support	2	3	1	4	2	3	1	5
Collaborative research	7	8	1	18	7	16	6	22
Personnel exchange	4	4	1	11	6	6	1	10
Financial support	8	4	1	19	6	7	3	14
In-kind contribution	4	5	1	10	4	4	1	6
Facilities	4	3	1	9	5	9	2	16
Unknown	7	5	1	13	3	11	2	26
Student training/career development	3	1	1	1	4	3	1	5
K-12 education	2	3	2	3	2	1	1	1
General public outreach	1	2	2	2	2	3	1	5
Other	1	1	1	1	0	0	0	0

Sources: Phase I and Phase II Annual Reports from Phase I/II CCIs between 2004 and 2016 – Participants/Organizations.

Additional information related to industrial partnerships was available from non-center-generated administrative records. In early years, several centers were encouraged to increase both the number of partners and the extent of interactions with them, but the views of Site Visitors about partnerships appeared to have improved over time. In one center, Site Visitors praised a robust industry affiliates program, which provided new research opportunities, led to instrument development, and offered pathways for commercialization. Site Visitors for another center noted that the CCI-industry partner relationships were clearly defined and that the center had put in place a management approach that could accommodate a range of industry requirements. Finally, some Site Visitors made positive comments about the diversity of industry representation on the advisory boards.

> *"It is clear that there are significant, bidirectional benefits that derive from these relationships [with the network of industrial partners, sponsors, and affiliates], which range from providing invaluable training and career development opportunities to students, to facilitating the adoption of … methodologies in industrial settings, and accelerating the Center's research by sharing expertise and instrumentation."*
>
> *–Site Visit Report*

Industry Partners derived many benefits from their affiliation with the CCI Program

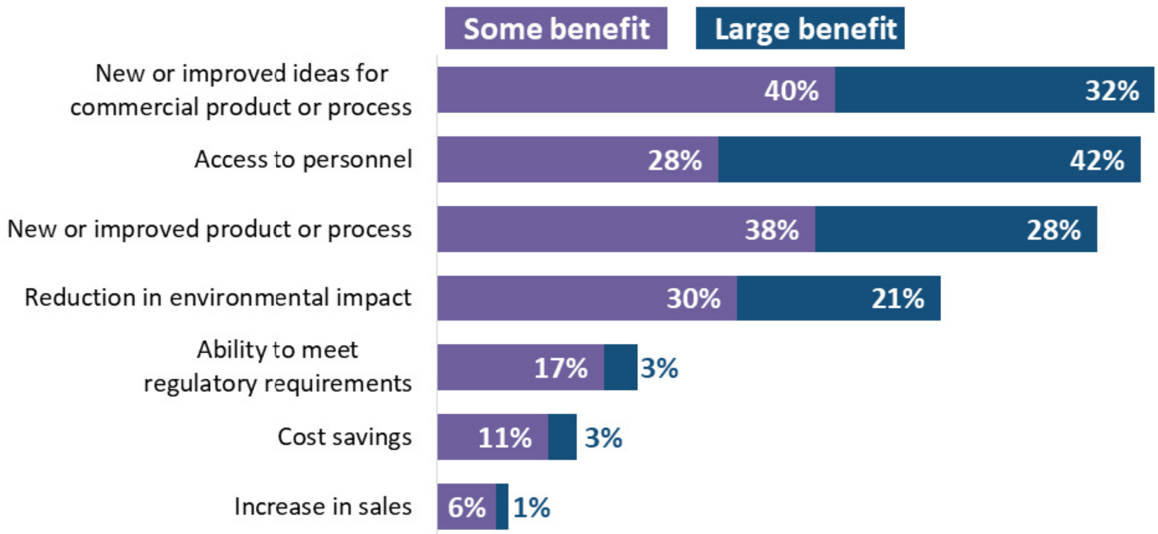
In the survey, PIs and Co-Investigators reported that commercial partners benefited from CCIs. These benefits included new or improved ideas for commercial products or processes (some or large benefit indicated by 72 percent of CCI investigators), access to personnel (70 percent), new or improved products or processes (66 percent), reduction in environmental impact (51 percent), ability to meet regulatory requirements (20 percent), cost savings (14 percent), and increase in sales (7 percent; Exhibit 18).

Furthermore, a survey of graduate students and postdocs revealed that participation in the CCI Program contributed to increased interest in working in industry and in commercialization among these groups.

Among the survey respondents, 13 percent indicated that they had participated in entrepreneurship (Exhibit 20) and 44 percent believed that learning about commercialization and entrepreneurship was an advantage (Exhibit 22). For about one-third of graduate students (33 percent) and one-fifth of postdocs (22 percent), a position in industry became a goal since their involvement in CCI (Exhibit 24).

An increase in relationships with industry was not limited to students. In the survey of CCI investigators, 31 percent also indicated greater interest in commercialization resulting from program participation; a smaller percentage received funding from (15 percent) and published with (13 percent) an industry partner (data not shown).[45]

Exhibit 18: Benefits of CCI to Industry include Ideas, Staff, Products, and Reduction in Environmental Impact



Note: N = 134, missing = 5–12. Two response options are not displayed: "No benefit due to CCI" and "Uncertain." For a table with all response options, see Appendix H, Exhibit H-11.

Source: Survey of Principal Investigators and Co-Investigators Q14 (Please indicate whether the CCI delivered any of the following benefits to industry.).

45 Appendix H, Exhibit H-6, presents complete information for this survey item.

Chapter 5: Research Question 3 Findings

RQ 3: What are the contributions of the CCI Program in the areas of workforce development (education and professional development), broadening participation, and informal science communication?

Sub-Question	Extent Addressed	Comment
3.1 What are the most important impacts of the CCIs in these three areas and how was this made possible (or enhanced) by the center mechanism of operation?	●	Fully addressed in this chapter
3.2 To what extent and in what ways are the CCIs providing leadership in these three broader impact areas?	○	Unable to operationalize leadership
3.3 To what extent and in what ways have the CCIs contributed to sustained, institutionalized change in these three broader impact areas?	◐	Unable to quantify institutional change

Sub-question 3.1. What are the most important impacts of the CCIs in these three areas and how was this made possible (or enhanced) by the center mechanism of operation?

Workforce Development

Based on the data reported by the centers, an average of 7 undergraduates, 11 graduate students, and 4 postdocs participated per Phase I center per year; and an average of 20 undergraduates, 38 graduate students, and 19 postdocs participated per Phase II center. We describe their experiences in this section. CCIs also launched numerous programs to increase the representation of women and minorities in STEM and to interest the public in science, which are presented separately below.

CCIs launched many programs to improve the student experience

In the survey, the majority of CCI investigators reported that the centers developed or improved various educational opportunities, including courses and seminars in chemistry (63 percent), training programs (61 percent), and research and teaching experiences (88 percent, data not shown).[46] Moreover, respondents to this survey believed that the centers brought about improvements in the quality of education in chemistry (83 percent) and helped graduate students and postdocs obtain a position after leaving the center (85 percent, data not shown).[47]

A review of center documents and interviews with CCI PIs and Managing Directors provided numerous examples of professional development opportunities. These included lectures, courses, seminars, and summer schools focused on a particular topic in chemistry or a related field. For example, one center mentioned a three-day summer school in Raman spectroscopy, which attracted more than 70 participants, including 40 not affiliated with the center. Another described a fabrication laboratory where students could learn to manufacture instruments. All centers offered students, including undergraduates, an opportunity to get involved in research projects both during the academic year and over the summer.

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46 Appendix H, Exhibit H-8, presents complete information for this survey item.

47 Appendix H, Exhibit H-10, presents complete information for this survey item.

One of the unique aspects of the CCI Program that emerged from the documents and the investigator survey was an emphasis on collaborative experiences. Centers encouraged students and postdocs to work at other institutions through a "Researcher in Residence" program (an exchange program with the University of Edinburgh), industry internships, and similar programs. In addition, center-wide meetings and seminars offered students and postdocs opportunities to share their work so that they can receive feedback from peers and faculty, and form connections. These junior scholars were also offered travel grants and other financial support to attend and present at national meetings, such as the American Chemical Society and Gordon conferences.

Annual reports described many events hosted by CCIs that focused on career development. These covered topics such as traditional and alternative career paths for chemists; entrepreneurship and commercialization; work-life balance; budget, project, and personnel management; proposal writing; team-building and collaboration; diversity; and leadership. CCIs also offered to hone the skills of communicating science to technical and general audiences, such as workshops on storytelling and effective oral presentations. One center developed a "Guide to Authorship" for its participants.

Examples of Career Development Workshops:

- *Preparing Future Innovators seminar series*
- *Chemistry Careers seminar*
- *Networking Strategies workshop*
- *Postgraduate Career Strategies webinar series*
- *Chemistry Resume workshop*
- *Career Interview Skills workshop*

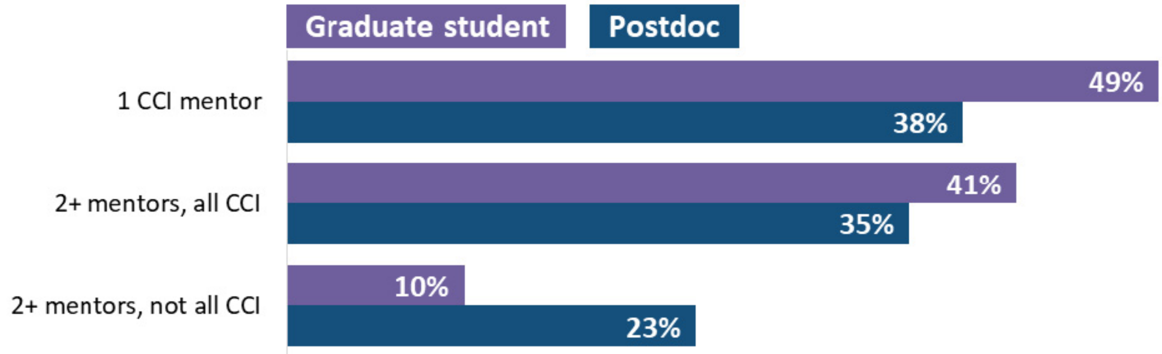
According to center documents, many CCIs also provided their students with leadership opportunities. Some CCIs had student-led councils responsible for organizing workshops and social events, providing input on student interest in center initiatives, and serving as liaisons between students and center management. In one center, students could apply for seed grants to fund collaborative research with two or more center members, so that they could practice proposal writing and project planning. In another, students founded a Women in Chemistry organization to bring female scientists together. Finally, most centers reported activities related to teaching. These included developing and teaching laboratory courses for undergraduates based on the center research and working with K-12 schools to develop science curricula.

In interviews, CCI PIs and Managing Directors expressed pride in their professional development programs, which they believed produce exceptional, well-rounded students connected to strong peer and faculty networks, who had acquired the skills not typically taught in graduate school.

Student mentoring was an important component of all CCIs

In the survey of graduate students and postdocs, we explored the topic of mentorship, which is instrumental to positive training experience. The data revealed that 58 percent of graduate students and 51 percent of postdocs had multiple mentors (Exhibit 19), of which at least one was affiliated with CCI. Being connected to more than one faculty member helps students in large laboratories, and provides an outlet for those who do not get along with their primary advisor. In an interview, one CCI PI said that having multiple mentors (which is the case for all students in their center) helped the students be more interactive and better prepared for their next career stage. Many examples of mentorship activities were also described in center documents. These included research guidance, and help with resumes, job searches, and interviews.

Exhibit 19: More than Half of Graduate Students and Postdocs had multiple Mentors



Notes: Graduate student (N = 227, missing = 0), postdoc (N = 113, missing = 0), overall (N = 340, missing = 0). Two response options are not displayed: "I have a single mentor who does not participate in CCI" and "I do not have any mentors." For a table with all response options, see Appendix I, Exhibit I-4.

Source: Survey of Current and Former Graduate Students and Postdocs Q7 (How many people served as mentors to you (either formally or informally), providing guidance, feedback, and support for your development and research?).

External perspective on student professional development

Site Visitors expressed very positive views about student professional development opportunities, highlighting mentorship, collaborative funding programs, laboratory exchanges, involvement in curriculum development, training in science communication, and activities to learn about and get involved with industry. CCIs were also praised for successfully placing students and postdocs in jobs in industry, national laboratories, and academia. The most frequent recommendation for improvement was to create professional development plans and provide more explicit guidance on how to contribute to center goals and balance time between research and non-research activities. One center was advised to better integrate undergraduates in the center research.

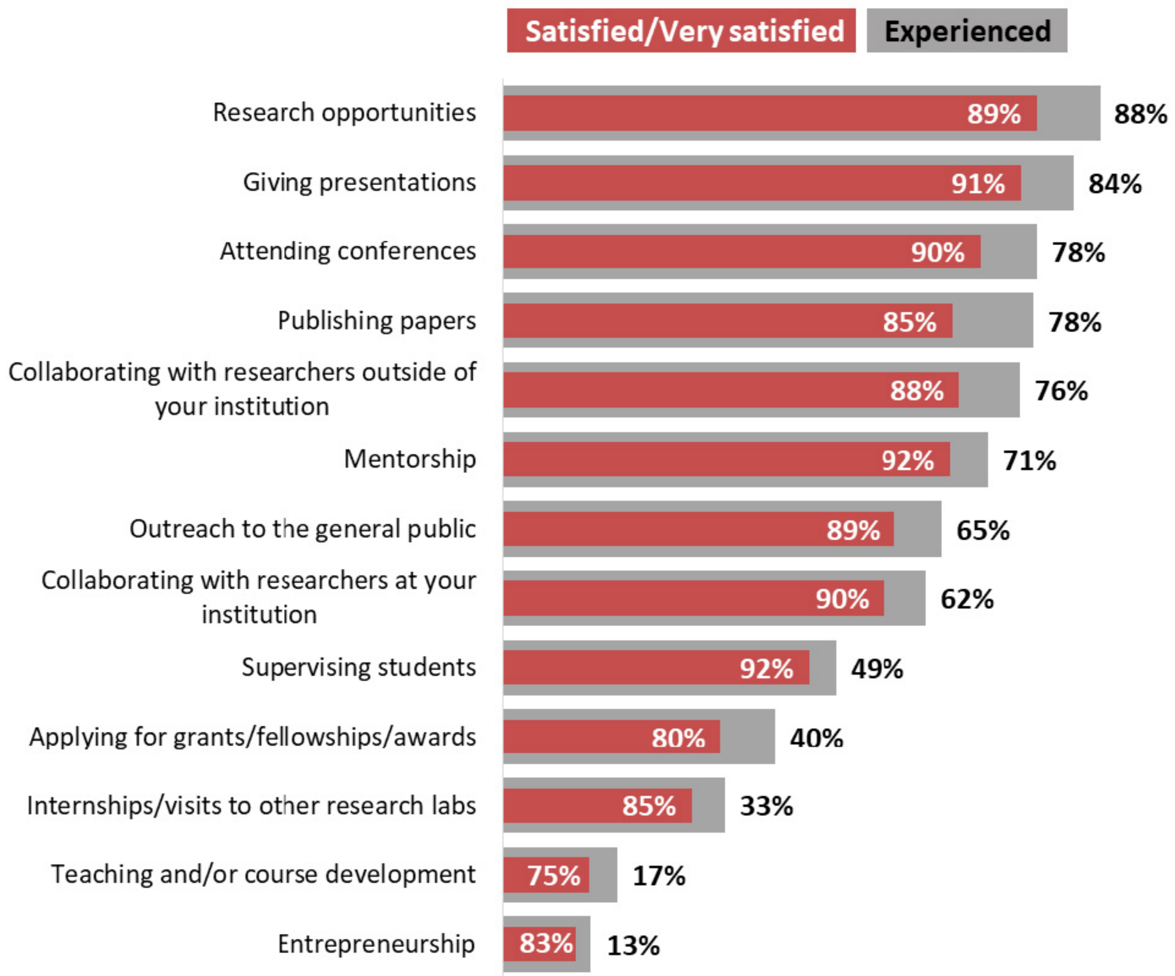
> *"Collaborative interdisciplinary opportunities and professional development activities enabled by the Center are exemplary."*
>
> *–Site Visit Report*

In interviews, Industry Partners and Site Visitors confirmed that they viewed student development and public education as important and successful components of the centers. These respondents believed that taxpayer dollars were well spent on inspiring the next generation of scientists and on raising the understanding of basic research among the public. One Site Visitor praised CCI students for their maturity, level of engagement in the center, and scientific knowledge.

Students confirmed that they benefited from CCI participation

In the survey, graduate students and postdocs affiliated with CCIs reported that they had access to a broad range of opportunities. Most commonly mentioned were conducting research (88 percent), presenting their work and publishing papers (84 percent and 78 percent, respectively), attending conferences (78 percent), being mentored and serving as mentors (71 percent and 49 percent), participating in public outreach (65 percent), and collaborating with researchers at and outside of their institution (62 percent and 76 percent, Exhibit 20). A third or fewer participated in internships or visits to center partners (33 percent), teaching or course development (17 percent), or entrepreneurship (13 percent). Among the survey respondents who took part in various opportunities, three-quarters or more were satisfied or very satisfied with these experiences (Exhibit 20),[48] and 90 percent with the CCI overall (data not shown).[49] The reasons for the dissatisfaction articulated by 11 respondents included inadequate leadership or mentorship, the environment in their group, collaborators, or having too much to do (data not shown).

Exhibit 20: Graduate Students and Postdocs were Satisfied with a Broad Range of Career Development Opportunities Available at CCIs



Notes: Q13 N = 340, missing = 0; Q14 N = 50–300, missing = 0–3.

Sources: Survey of Current and Former Graduate Students and Postdocs Q13 (Which of the following professional development opportunities offered through your CCI have you experienced?), Q14 (How satisfied are you with these opportunities?).

Responses for Q13 may not sum to 100% because multiple responses were permitted. Responses for Q14 are limited to respondents who indicated the professional development opportunity was offered through their CCI in Q13. Inner bar values are expressed as a percentage of the corresponding outer bar.

Survey data also revealed that 76 percent of graduate students and postdocs collaborated with researchers outside of their institution,[50] and 23 percent worked in a laboratory at a CCI partner organization[51] (data

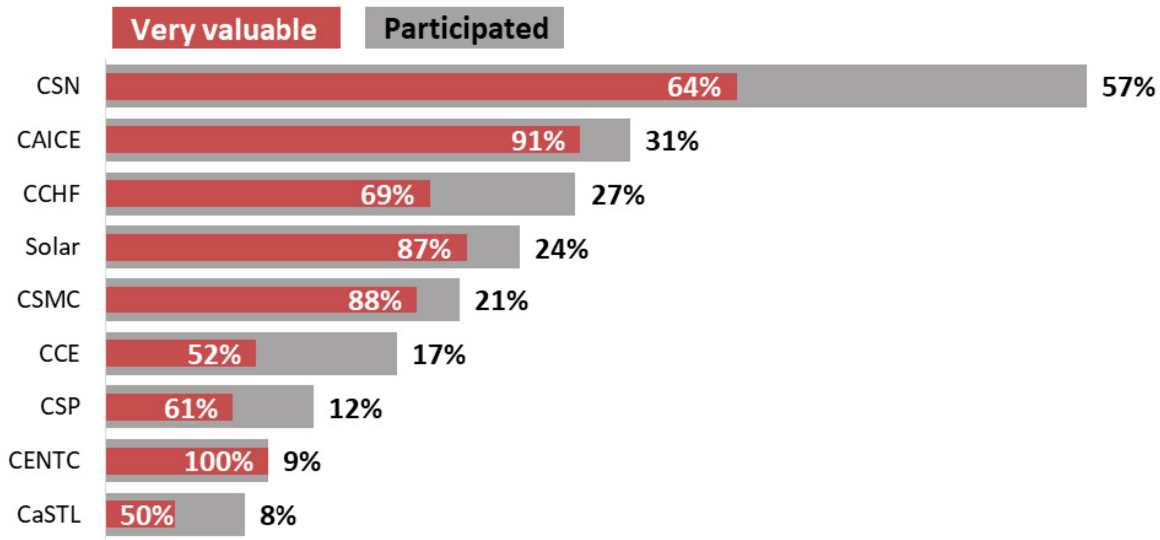
48 Only 6 percent or fewer of participants were dissatisfied or very dissatisfied with any of the experiences.

49 Appendix I, Exhibit I-12, presents complete information for this survey item.

50 Appendix I, Exhibit I-10, presents complete information for this survey item.

not shown). Depending on the center, between 8 percent and 57 percent made these visits, and among these half or more found the experience very valuable (Exhibit 21).[52] Ninety-one percent of hosting organizations were universities[53] and the duration of the visit for 70 percent of students and postdocs was less than three months (data not shown).[54]

Exhibit 21: Most Graduate Students and Postdocs Who Worked at a Partner Organization Found the Experience Very Valuable



Note: CAICE (N = 10, missing = 0), CCE (N = 4, missing = 0), Solar (N = 7, missing = 0), CENTC (N = 5, missing = 1), CCHF (N = 13, missing = 0), CSMC (N = 9, missing = 0), CSN (N = 28, missing = 0), CSP (N = 5, missing = 0), CaSTL (N = 2, missing = 0), overall (N = 83, missing = 1). Listed center is the graduate student or postdoc's home center.

Sources: Survey of Current and Former Graduate Students and Postdocs Q12 (Have you spent time working in a laboratory/research group of another CCI partner organization (e.g., another university or company involved with your center) as an intern, graduate student, visiting scholar, or similar role?); Q12C (How valuable was this experience to your career development?). Inner bar values are expressed as a percentage of the corresponding outer bar.

In the survey, graduate students and postdocs were asked whether various opportunities to which they had access through CCI had proven to be an advantage to their careers and, if yes, in what way. The vast majority indicated that they benefited from the breadth of research experience and from exposure to scientific areas outside of their own field (94 percent and 82 percent, Exhibit 22). Other commonly reported advantages were access to a community of peers (88 percent), faculty (78 percent), and equipment/facilities/materials/reagents (78 percent). Being part of CCI enabled participants to advance their research projects (82 percent), take on leadership responsibilities (69 percent), develop their own ideas (64 percent), and learn how to communicate about their work (82 percent). Finally, CCI participation helped many graduate students and postdocs explore various career options (63 percent) and improved their access to job opportunities (53 percent). A majority of graduate students and postdocs

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[51] Appendix I, Exhibit I-9, presents complete information for this survey item.

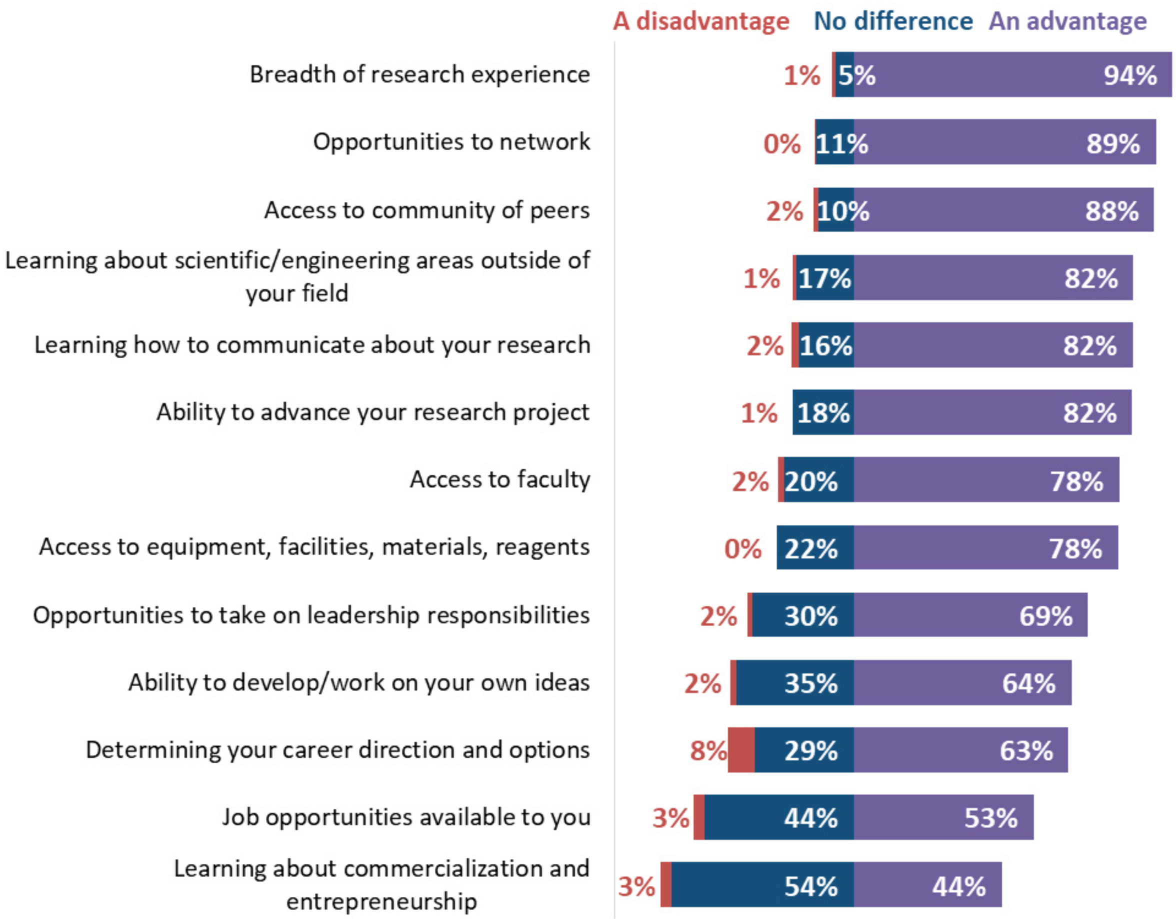
[52] The remaining graduate students and postdocs found their experiences at partner organizations somewhat valuable or reported it was too early to tell. None reported that the experience was not at all valuable.

[53] Appendix I, Exhibit I-9a, presents complete information for this survey item.

[54] Appendix I, Exhibit I-9b, presents complete information for this survey item.

(57 percent) reported that CCI either made no difference or was a disadvantage for learning about commercialization or entrepreneurship.

Exhibit 22: Professional Development Opportunities Available at CCIs Were an Advantage



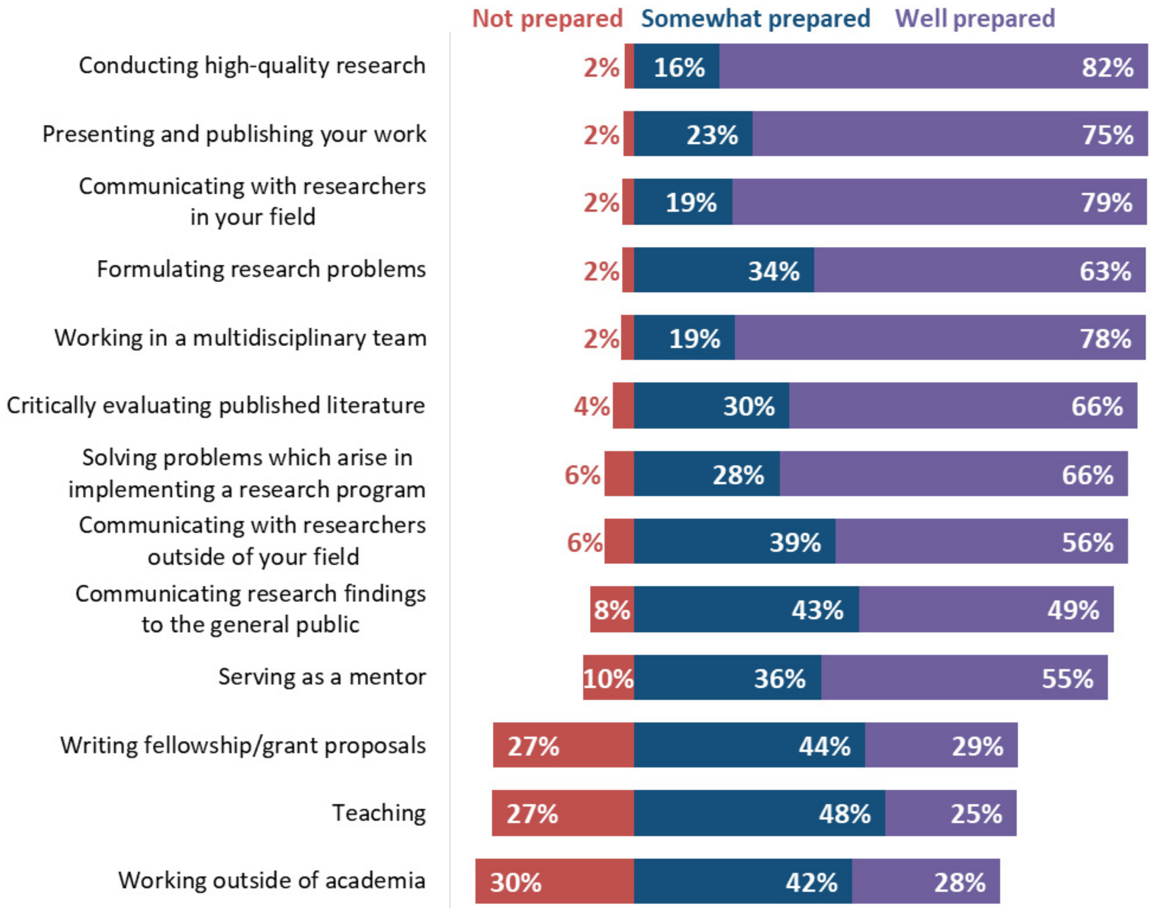
Notes: N = 340, missing = 2–3, not applicable/too early to tell = 2–33.

Source: Survey of Current and Former Graduate Students and Postdocs Q16 (Please indicate, for each item below, whether participation in CCI has proved to be an advantage, disadvantage, or made no difference).

Graduate students and postdocs responding to the survey said that CCI participation furnished them with many competencies important to a career in or outside of academia. The experience prepared them to conduct high-quality research (82 percent), communicate with researchers within and outside of their field (79 percent and 56 percent), work in a multidisciplinary team (78 percent), present and publish their work (75 percent), critically evaluate published literature and formulate research problems (66 percent and 63 percent, solve problems (66 percent), and serve as mentors (55 percent; Exhibit 23). CCI participation was less helpful for developing skills in proposal writing (29 percent), working outside of academia (28 percent), and teaching (25 percent). Two-thirds said that being part of CCI improved the quality of their education and training (data not shown).[55]

[55] Appendix I, Exhibit I-13, presents complete information for this survey item.

Exhibit 23: CCI Prepared Graduate Students and Postdocs for Research Careers



Notes: N = 340, missing = 3–7, not applicable/too early to tell = 8–52.

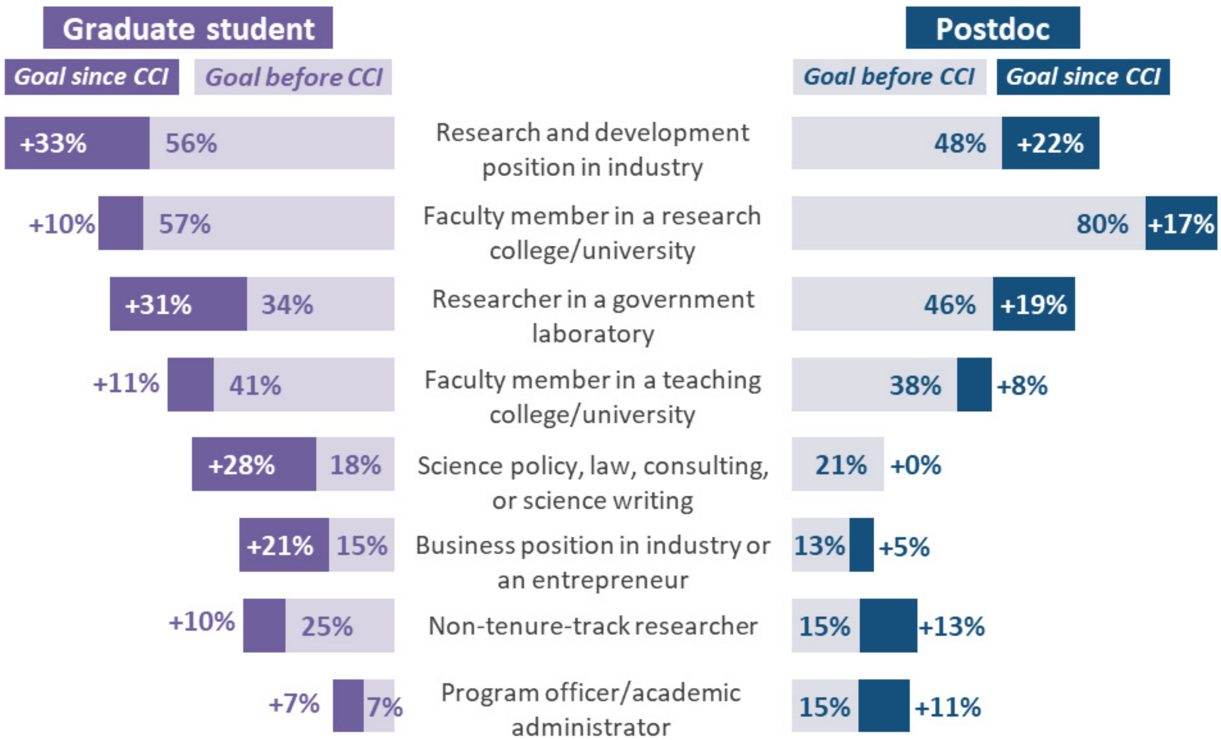
Source: Survey of Current and Former Graduate Students and Postdocs Q17 (How well do you think participation in the CCI is preparing you for the following activities?).

CCI influenced career choices made by graduate students and postdocs

Many graduate students and postdocs reported having clear career aspirations before joining CCI, but some became interested in additional types of positions after being affiliated with the center. Prior to CCI, the most common goal for postdocs was a faculty position in a research college or university, indicated by 80 percent of respondents, with a research and development position in industry or a government laboratory by 48 and 46 percent, respectively (Exhibit 24). Less than 40 percent of postdocs were interested in a faculty position in a teaching college, and less than 25 percent in non-tenure track research positions as well as in positions in law, science policy, academic administration, and other alternative career paths often pursued by scientists. Responses from graduate students were similar, but showed less commitment to a faculty track at a research college or university (57 versus 80 percent).

After joining a CCI, an additional 33 percent of graduate students became interested in a research position in industry; 31 percent in a government laboratory; 28 percent in science policy, law, consulting, and science writing; and 21 percent in a business position or entrepreneurship (Exhibit 24). Approximately 10 percent became more interested in a faculty position, a non-tenure researcher position, or a program officer/academic administrator position. Postdocs were less likely to want to change career goals than students, especially to alternative careers (Exhibit 24).

Exhibit 24: CCI Prompted Some Graduate Students and Postdocs to Change Their Career Goals

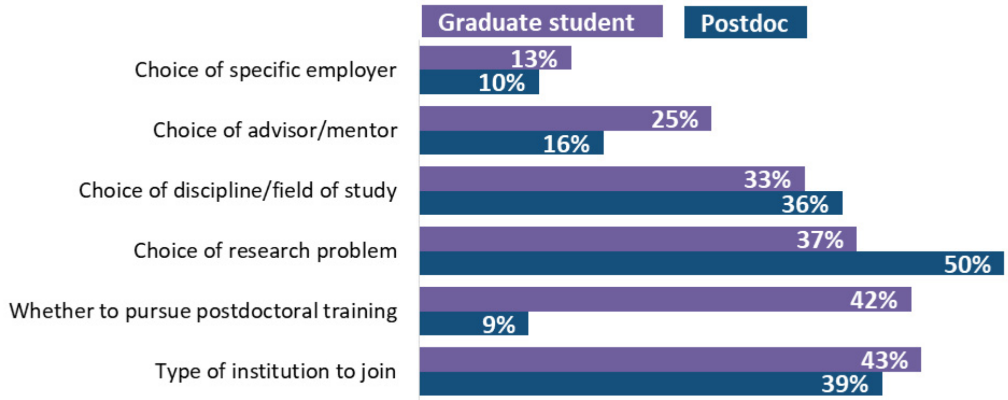


Note: Graduate student (N = 82, missing = 0–6), postdoc (N = 18, missing = 0–2). Limited to current students.

Source: Survey of Current and Former Graduate Students and Postdocs Q11 (Which of the following positions are you most interested in pursuing after you complete your degree and/or postdoctoral training? Have your career goals changed since you began participating in the CCI?).

CCI participation influenced career-related choices of graduate students and postdocs beyond the types of positions. These included the type of institution to join (43 percent of graduate students and 39 percent of postdocs); whether to pursue postdoctoral training (42 percent and 9 percent); as well as the choice of research problem (37 percent and 50 percent), discipline (33 percent and 36 percent), and advisor/mentor (25 percent and 16 percent; Exhibit 25). Postdocs again emerged as more established in their choices.

Exhibit 25: For Many Students and Postdocs, CCI Influenced the Choice of Institution, Problem, Field of Study, and Advisor



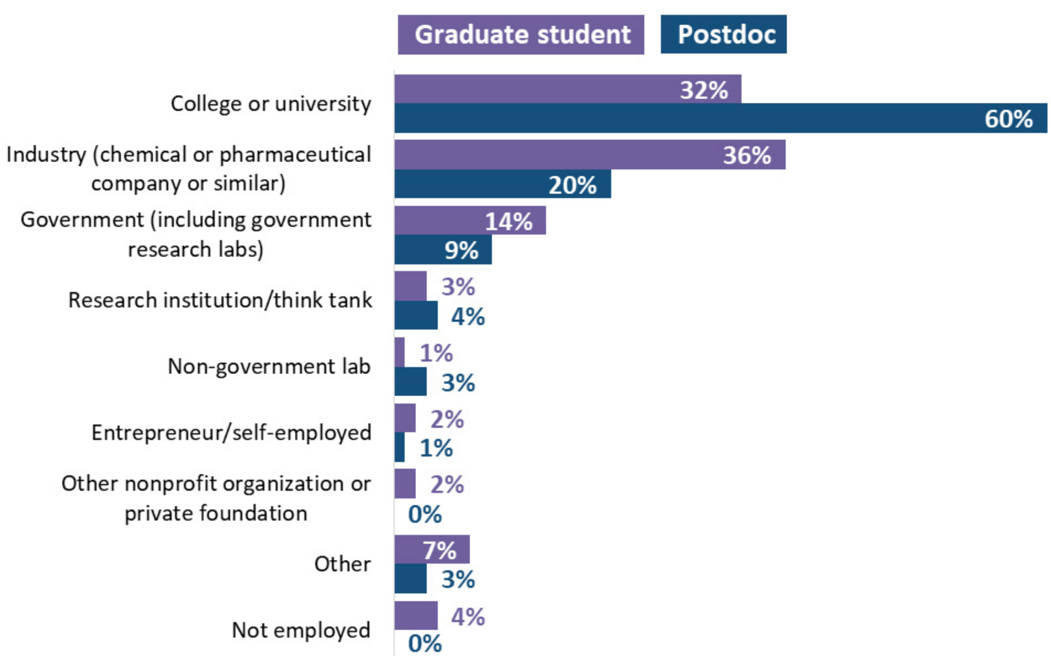
Note: Graduate student (N = 145, missing=0), postdoc (N = 95, missing = 0).

Source: Survey of Current and Former Graduate Students and Postdocs Q8 (Did your CCI experiences influence any of these choices?). Responses may not sum to 100% because multiple responses were permitted. Responses were limited to past students.

Former CCI graduate students and postdocs are employed in a variety of organizations

Employment of CCI alumni was consistent with their career goals: 36 percent of former graduate students and 20 percent of postdocs reported having a position in industry; and 32 percent and 60 percent at a college or university, respectively (Exhibit 26). Relatively few reported working for the government (14 percent of graduate students and 9 percent of postdocs), and even fewer were employed by other organizations, self-employed, or unemployed (4 percent or less).

Exhibit 26: Most Former Graduate Students and Postdocs Were Employed in Academia or Industry



Note: Graduate (N = 126, missing = 0), postdoc (N = 94, missing = 0).

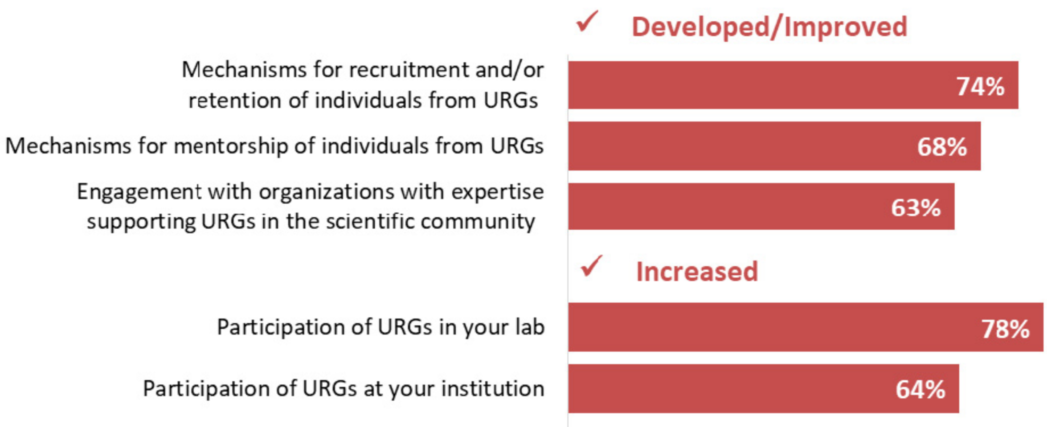
Source: Survey of Current and Former Graduate Students and Postdocs Q10 (Which of the following best describes your current principal employer?) Responses were limited to past students not currently enrolled in a degree program.

Broadening the Participation of Underrepresented Groups in STEM (URGs)

CCIs developed many mechanisms and programs to broaden participation, but it is not clear whether this led to an increase in the representations of URGs

In the survey, CCIs investigators indicated that the program contributed to the NSF's mission of broadening participation of URGs by developing or improving recruitment, retention, and mentorship mechanisms (reported by 68 to 74 percent of respondents) and through engagement with organizations that support URGs (reported by 63 percent of respondents; Exhibit 27). Furthermore, most CCI investigators believed that these activities increased the diversity of their own laboratory (78 percent) and institution (64 percent) and contributed to the success of their center (98 percent, data not shown).

Exhibit 27: CCIs Developed or Improved Mechanisms to Support URGs Which They Viewed as Effective



Note: Q11 (N = 134, missing = 0), Q13 (N = 134, missing = 4–6); Q16 "Broadening Participation" (N = 123, missing = 11).

Sources: Survey of Principal Investigators and Co-Investigators Q11 (Please indicate whether your CCI developed or improved the following educational and/or outreach opportunities.). Q13 (Please indicate whether the following improvements have occurred as a result of CCI funding). Q16 (To what extent have these elements contributed to the success of your center?).

Center documents revealed that CCIs targeted URGs at all educational stages. For example, graduate students at one CCI visited K-12 schools on a bimonthly basis to conduct interactive science experiments, mentor students, and encourage them to attend college. Other centers invited K-12 students to visit their laboratories and spend time on a college campus. Several programs were specifically developed for female students from underserved regions. For example, one center organized activities that brought together CCI female students and middle school girls, and another partnered with a local television station that produced a girls' science television show.

Examples of Activities to Broaden Participation:

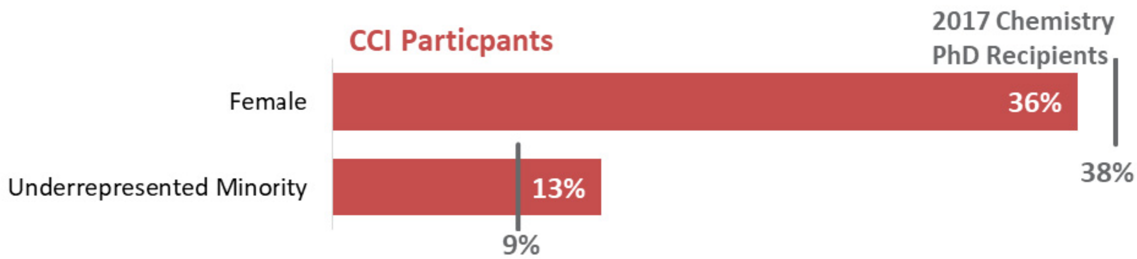
- *Partnered with local community college to bring science kits and solar energy concepts to hundreds of underserved minority students along the U.S.-Mexico border*
- *Developed sabbatical programs for faculty at Puerto Rican universities to visit a continental U.S.-based university to build research connections*
- *Provided first generation, economically disadvantaged students with the opportunity to participate in a summer science research project*
- *Conducted annual surveys focused on center climate, including issues of diversity*
- *Embedding topics related to diversity in weekly center-wide presentations*
- *Sponsored an undergraduate HBCU club focused on career development*

To recruit minority students, CCI staff attended events hosted by the Society for the Advancement of Chicanos/Hispanics and Native Americans in Science, the Annual Biomedical Research Conference for Minority Students, and similar professional organizations. CCIs also formed partnerships with Historically Black Colleges and Universities (HBCUs), and similar organizations to foster collaboration with faculty and to create student research and other career development opportunities.

In addition to these outreach activities, CCIs provided supports to minority students at the centers. These included a "buddy" program, where graduate students and postdocs from URGs served as mentors for undergraduates, and an on-boarding committee to help integrate new minority students. Finally, CCIs encouraged students from URGs to participate in NSF research programs, such as the Research Experience for Undergraduates.

To determine whether these efforts were reflected in the demographic composition of CCI graduate students and postdocs, we examined the gender and racial/ethnic minority status of graduate student/postdoc survey respondents. We found that 36 percent identified as female and 13 percent as racial/ethnic minorities (Exhibit 28). We compared these data to the national sample of chemistry doctorate recipients in 2017 and found that CCI participants were slightly less likely to identify as female (36 versus 38 percent), but more likely to identify as an underrepresented minority (13 versus 9 percent). We note that only about half of graduate students and postdocs responded to the survey, leaving open the possibility that these demographic statistics do not accurately represent the CCI community.

Exhibit 28: Representation of URGs at CCIs Was Similar for Gender and Slightly Better for Racial/Ethnic Diversity than National Averages



Note: N = 340, missing = 2.

Sources: Survey of Current and Former Graduate Students and Postdocs Q18 (What is your gender?); Q19 (Do you identify as an underrepresented ethnic/racial minority?); NSF, Survey of Earned Doctorates, doctorate recipients, by sex and major field of study: 2008–17 (Table 15); NSF, Survey of Earned Doctorates, U.S. citizen and permanent resident doctorate recipients, by major field of study, ethnicity, and race: 2017 (Table 24).

Site Visitors provided positive perspectives on efforts to broader participation but asserted that more work needed to be done

Site Visitors provided many positive comments on CCI efforts to build recruitment pipelines, engage community organizations, and reach out to peers for ideas. At some centers, they also noted that PIs and Co-Investigators offered seemingly effective mentoring and other support to students from diverse backgrounds. However, site visit reports recommended that CCIs try to improve the diversity of the center faculty, especially among the leadership. Another common suggestion was to better articulate diversity goals and plans to achieve them.

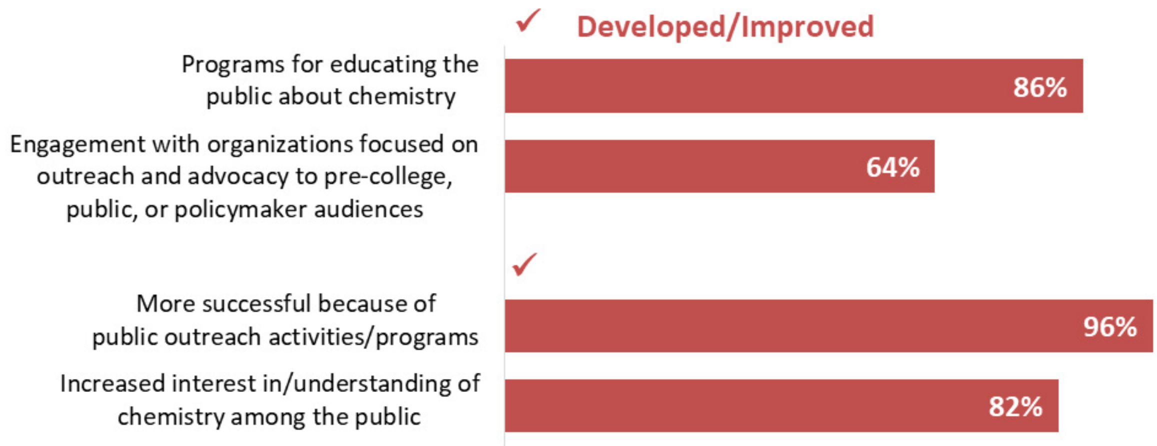
> *"The inclusion of HBCUs and PUIs [Primarily Undergraduate Institutions] is a real strength of the [Center] that adds value in progress toward the scientific, education and outreach goals of the Center. The committee values the participation of high school students and teachers in scientific programs and encourages expansion of high school participation across the [Center]."*
>
> *–Site Visitor*

Promoting the Public Understanding of Science

CCIs created many programs for educating the public about chemistry

Nearly all PIs and Co-Investigators (86 percent) reported developing or improving programs to educate the public; and 64 percent partnering with organizations focused on outreach and advocacy to pre-college, public, or policymaker audiences (Exhibit 29). Furthermore, 96 percent of PIs and Co-Investigators said that these efforts contributed to the success of their center to some or a considerable extent, and 82 percent said that CCIs led to some or large improvements in the interest and understanding of chemistry among the public.

Exhibit 29: CCIs Established Many Programs to Educate the Public about Chemistry Which They Viewed as Effective



Note: Q11 (N = 134, missing = 0), Q13 (N =134, missing = 4–6), Q16 "Public Outreach" (N = 122, missing = 12).

Sources: Survey of Principal Investigators and Co-Investigators Q11 (Please indicate whether your CCI developed or improved the following educational and/or outreach opportunities.). Q13 (Please indicate whether the following improvements have occurred as a result of CCI funding). Q16 (To what extent have these elements contributed to the success of your center?).

A review of CCI center documents produced numerous examples of outreach programs. These included hosting or participating in science festivals, symposia, and workshops; giving demonstrations using science kits and portable experiments; serving as judges at science fairs or poster competitions; designing museum exhibits and science booths; and giving public presentations and lectures. In order to reach broader audiences, some of these outreach efforts occurred in cafes, theaters, slam poetry shows, breweries, parks, senior/retirement communities, rotary clubs, and business offices. CCIs formed many community partnerships to enhance these efforts. CCIs also took advantage of a broad range of dissemination modalities, which included websites, web tutorials, Facebook and Twitter postings, podcasts, radio shows, and blogs. For example, one CCI collaborated with a science journalist from National Public Radio to create a series of stories about chemistry. Another center launched a YouTube channel and started a science blog for Spanish speakers.

Examples of Outreach Activities:

- *Collaborated with the Oregon Museum of Science and Industry to engage the public with demonstrations*
- *Partnered with a botanical garden in a summer series*
- *Produced a show about chemical evolution*
- *Displayed exhibits for the Discovery Science Center*
- *Produced visual art pieces that were placed on trains*
- *Hosted interactive activities at large public events, such as the San Diego Science and Engineering Festival Expo Day*

All CCIs created programs that targeted K-12 students. These included laboratory tours, research

Examples of Activities Targeting K-12 Students:

- *Visited high schools to promote science careers as part of "Ask-A-Scientist" program*
- *Disseminated "Solar Energy Activity Lab" kits to expose hundreds of students to research on solar fuels*
- *Hosted "Science Saturdays" program to introduce local high school students to contemporary research*
- *Offered mock crime scene investigations to introduce high school students to analytical methods to test for heavy metals*
- *Partnered with the Optical Society of America to develop "Spectroboxes" to teach children about the properties of light using simple household tools*

opportunities, and college/career guidance. Many of these offerings were available after school or in the summer. The centers also worked with teachers on developing curricula and other educational aids. For example, one CCI created a video that depicted the dynamic nature of molecular matter to replace a static textbook picture, and another created games for children focused on basic science.

In interviews, PIs and Managing Directors explained that they focused on K-12 students because they believed in the importance of engaging young children to "prime the pipeline." Specific examples of these activities highlighted in interviews with PIs and Managing Directors included collaborations with local museums and youth development organizations (such as 4-H) to disseminate information about science and a blog launched and run by CCI students, which had been linked to many popular internet sites, and which led to an invited talk about the blog at an international conference. One CCI described their very successful outreach effort called "the Solar Army," which they believed should be used as a model for engaging the public. Solar Army now includes 3,000 high school students worldwide searching for new materials with kits fabricated by the center 20 years ago, as well as a long list of successful alumni. The program received numerous national awards and earned the already famous PI the title of "Solar General."

CCI PIs and Managing Directors also noted that these outreach activities were helpful to CCI students, who learned how to speak about science in non-technical language. Industry Partners and Site Visitors confirmed the contributions of CCIs to student development and public education, which they saw as important and successful components of the centers. They reported that taxpayer dollars were well spent on inspiring the next generation of scientists and on raising the understanding of basic research among the public. Numerous examples of these types of programs were also listed in annual reports.

"I'm very, very proud that we had real outreach that made a huge difference in human capital. We have literally hundreds of former mentors who are now in academic institutions all over the world as professors and we have them in industry and we have them in government. We have giant lists of successful people who were mentors in our Solar Army program and are now gone on to great things."

–CCI PI

"They view their role in the CCI as giant outreach and they have not been hesitant to share their model so that if other people want to climb on board and want to translate their outreach activities, their science events that they hold in their communities, they've been happy to share that information."

"It's very important for the public to understand what we're doing and why and why we're spending their tax dollars. We have a responsibility to do it."

–CCI Site Visitors

A few challenges related to public outreach also emerged. One Co-Investigator said that the work of his center was very fundamental and difficult for non-scientists to understand. Another mentioned that it was unclear what balance between outreach and research activities at CCIs was expected, and suggested that NSF provide more guidance about their expectations and the definition of progress. Finally, Site Visitors recommended that CCIs evaluate the effectiveness of their outreach programs to make more strategic choices. They also noted that outreach activities should be more evenly distributed across participants, including senior researchers. Finally, some oversight personnel indicated that their centers should extend their reach beyond K-12 programs and the local university community.

Sub-question 3.2. To what extent and in what ways are the CCIs providing leadership in these three broader impact areas?

While it was clear from the surveys and from interviews that CCI engage in numerous activities related to workforce development, broadening participation, and public outreach, we are uncertain how to characterize their leadership in these areas.

Sub-question 3.3. To what extent and in what ways have the CCIs contributed to sustained, institutionalized change in these three broader impact areas?

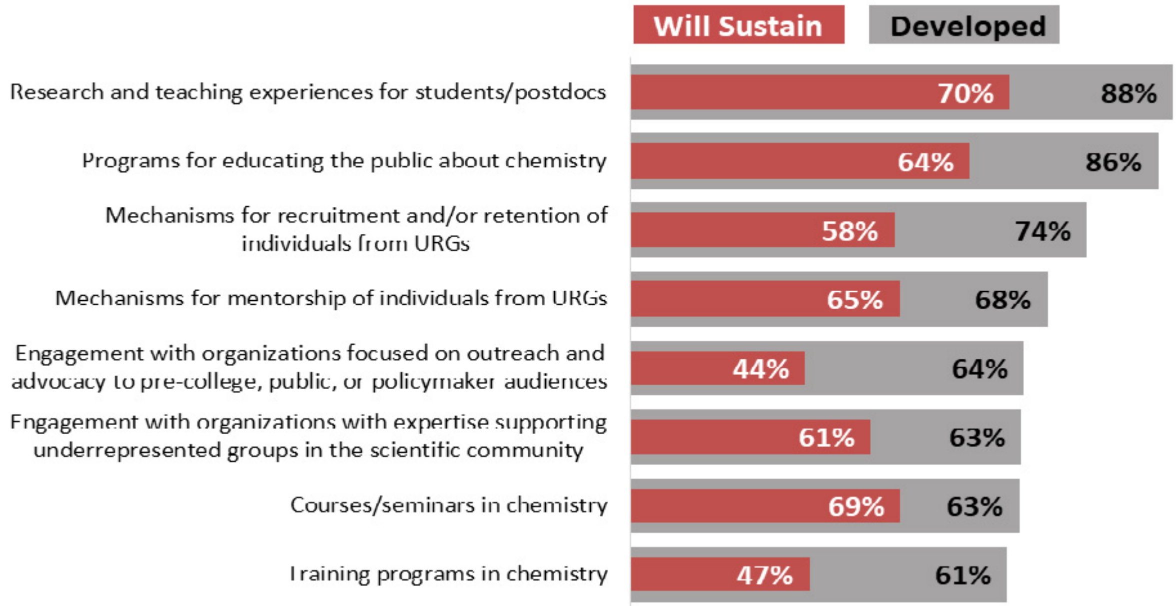
CCIs are leaving behind a lasting legacy, but many of their programs may not be sustainable

In the survey, 60 to 70 percent of CCI PIs and Co-Investigators indicated that research/teaching experiences, courses/seminars, public outreach programs, as well as mechanisms and partnerships to recruit and retain URGs developed by the centers would be sustainable after the end of the grant (Exhibit 30). These respondents were less confident about training programs in chemistry (47 percent) and partnerships with advocacy groups (44 percent).

We also explored the topic of sustainability in interviews with CCI PIs, Co-Investigators, and Managing Directors; and observed that they were less confident than survey respondents. Only one Managing Director said that their center had already secured some institutional funding and expected to be able to raise more from other sources, and thus many of their programs would probably continue. A few other respondents reported that their outreach programs or strategies were being adopted by their own or other universities. A few CCI PIs said that faculty at their centers had received or were applying for smaller multi-investigator awards or individual grants to continue with various research center projects, and one center was looking for funding to maintain its annual meetings. Simultaneously, two Co-Investigators were concerned about their ability to continue the work, and one of these Co-Investigators said that the STC of which he had been a member “scattered” after the grant ended, and so he was not very optimistic about the future of CCI. Some PIs wished that NSF played a larger role in the sunsetting process.

While many respondents did not think it would be possible to maintain the center or its components, all believed that CCIs would nevertheless leave behind lasting legacies. Examples of contributions that respondents reported would outlive or have outlived the centers cited in interviews included collaborations; new research directions taken by CCI participants; best practices for running a large center; companies based on CCI technologies; industry programs; videos, animations, and lesson plans; and students and postdocs who had “grown up” in the center.

Exhibit 30: CCI Investigators Believed that Many of Their Programs Will Be Sustained



Note: Q11 N = 134, missing = 0, Q12 N = 117, missing = 0.

Sources: Survey of Principal Investigators and Co-Investigators Q11 (Please indicate whether your CCI developed or improved the following educational and/or outreach opportunities.), Q12 (Please indicate whether you expect to be able to sustain the following programs and activities after the grant ends. If your grant has ended, please indicate whether these programs and activities are still in place.).

Responses for Q11 may not sum to 100% because multiple responses were permitted. Responses for Q12 are limited to respondents who indicated that the opportunity was developed or improved by their CCI in Q11. Inner bar values are expressed as a percentage of the corresponding outer bar.

We also explored the topic of sustainability with Industry Partners, Site Visitors, NSF staff, and PIs on non-CCI centers. Most Industry Partners expected their relationships with CCIs to continue, although none gave concrete examples of what form they would take. Site Visitors and NSF staff thought that it was unlikely that most centers would be able to continue their existence, especially if their work was not of immediate commercial interest. At the same time, these respondents spoke of the lasting impact of partnerships and collaborations, scientific contributions, students trained, and equipment. Finally, the sustainability expectations of non-CCI PIs for their centers were similar – they also described their legacies as new partnerships, workforce development, and leveraged support from new funders and donors. One Site Visitor argued that not all centers should be sustained. He said that it was productive for a group of researchers to get together and spend some time on an idea, but that the resulting science may not need a center environment to flourish. Somewhat similar views were expressed by a CCI PI, who argued that centers should have a finite lifespan, to allow other groups the same opportunities. This PI thought that 10 years was an appropriate duration for CCIs.

> *"The videos we are happy about and will have an indefinite lifetime. We tried to do them in a way where they are basic science and are not really speculative, so the content will remain true forever and they are so well done I don't see them getting outdated."*
>
> *–CCI PI*
>
> *"There will be other avenues besides single PI, but there is still a lot of concern if there will be enough money for all of us. How we will manage that will be a big issue for a lot of us."*
>
> *"The relationships may persist after the funding expires, but the rest of the structure probably not."*
>
> *–CCI Co-Investigators*

Chapter 6: Research Question 4 Findings

RQ 4: How effective are the centers' structures and operations in achieving the program's goals?

Sub-Question	Extent Addressed	Comment
4.1 What are some of the most effective center management strategies, and how are they adapted to their particular situations, in promoting (1) transformative outcomes, (2) enhanced team integration and augmented productivity (synergy), (3) higher quality training opportunities for students and postdocs, (4) increased diversity, and (5) improved public understanding and appreciation of chemistry?	●	Fully addressed in this chapter
4.2 To what extent and in what ways have the CCIs influenced collaborations among center participants?[56]	●	Fully addressed in this chapter
4.3 To what extent and in what ways have the CCIs made use of tools and communication to facilitate collaboration?	●	Fully addressed in this chapter

Sub-question 4.1. What are some of the most effective center management strategies, and how are they adapted to their particular situations, in promoting transformative outcomes, synergy, high quality training opportunities for students and postdocs, and improved public understanding and appreciation of chemistry?

CCIs were generally satisfied with partners, but challenges also existed

The ability to bring together teams of scientists with diverse expertise to approach a difficult problem is at the heart of the CCI Program. Therefore, the ability of the centers to effectively allocate and manage resources and to work together toward a common goal is instrumental to their success, and we examined these topics in depth.

In the survey, CCI researchers expressed mostly positive views about partnerships: 70 to 80 percent, depending on the item, were satisfied or very satisfied with the intellectual contribution of partners, communication tools, frequency and productivity of meetings, and distribution of resources (Exhibit 31A). Retention in the centers was also high, with 54 percent of survey respondents remaining affiliated for at least seven years and 95 percent for at least two years (data not shown).[57]

However, the survey also surfaced some challenges related to partnerships. Approximately 40 percent of PIs and Co-Investigators indicated challenges in terminating unsuccessful projects and communicating/coordinating with partners (Exhibit 31B). A smaller percentage were unsatisfied with accessing resources (17 percent), sharing of credit (21 percent), and with contributions of partners to the center (25 percent). However, virtually all of these challenges were resolved, likely contributing to the high level of satisfaction with the program, which was 86 percent (data not shown).[58]

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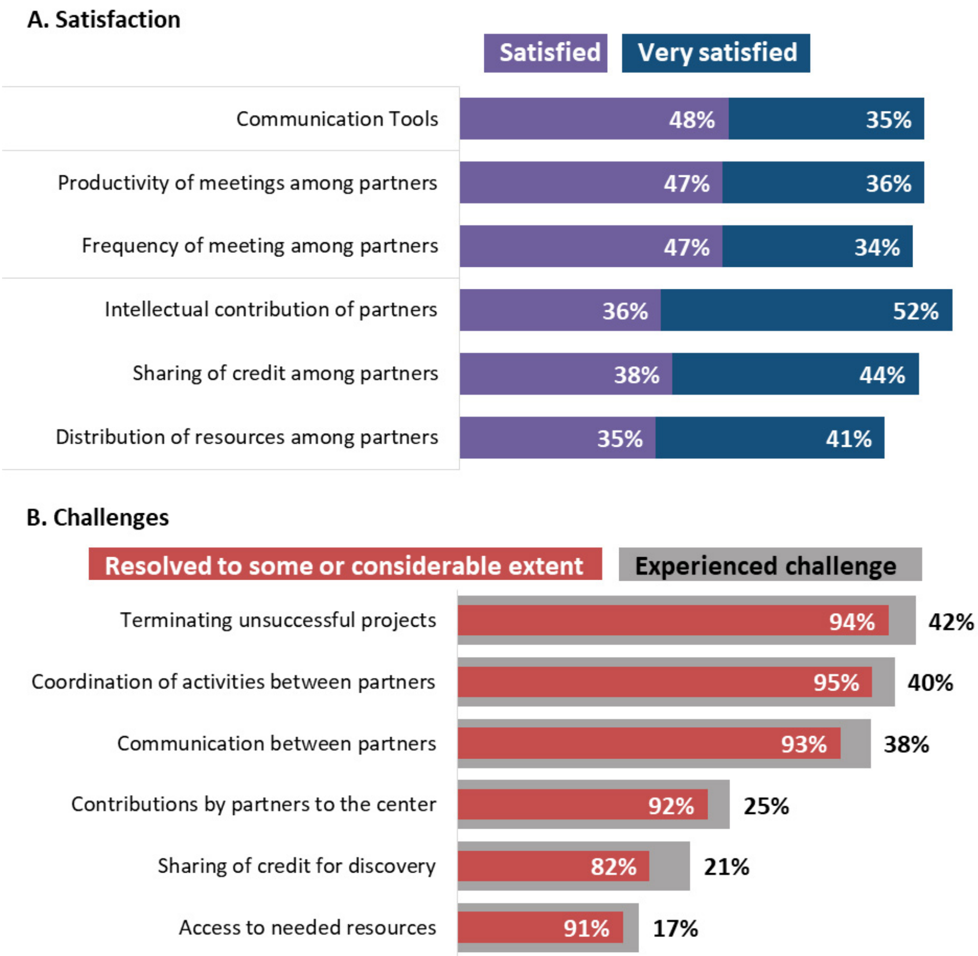
56 Research Question 4.2 was originally specified as: "To what extent and in what ways have the CCIs influenced and impacted collaborations among center participants?"

57 Appendix H, Exhibit H-1, presents complete information for this survey item.

58 Appendix H, Exhibit H-14, presents complete information for this survey item.

Additional insights about partnerships emerged from key informant interviews. When asked about the challenges in this area, CCI PIs and Managing Directors (as well as PIs for other NSF centers) most commonly talked about managing people. The problems included integrating participants with a range of interests and expertise into a cohesive research program, maintaining team engagement, and keeping all investigators focused of the mission of the center. Several CCI PIs also spoke about the importance of carefully assessing the true capability of each partner, setting goals that are concrete and are of interest to everyone in the center, articulating clear expectations, and providing frequent guidance and oversight. One center developed a detailed operational manual, which described the responsibilities of and expectations for all participants, which was viewed as very helpful by the PI.

Exhibit 31: CCI PIs and Co-Investigators Were Satisfied with the Partnerships and Were Able to Resolve Most Challenges



Note A: N = 134, missing = 5–22, N/A = 2–36. Three response options (in addition to N/A) are not displayed: “Very Dissatisfied,” “Dissatisfied,” and “Neutral.” For a table with all response options, see Appendix H, Exhibit H-12.

Source A: Survey of Principal Investigators and Co-Investigators Q15 (How satisfied are you with the following elements of CCI?).

Note B: Q18 N = 134, missing = 0; Q19 N = 79, Missing = 0–3.

Source B: Survey of Principal Investigators and Co-Investigators Q18 (Has your CCI experienced the following challenges?), Q19 (To what extent have these challenges been resolved?).

Responses for Q18 may not sum to 100% because multiple responses were permitted. Responses for Q19 are limited to respondents who indicated that the challenge had been experienced, according to Q18. Inner bar values are expressed as a percentage of the corresponding outer bar.

Despite the best efforts of PIs to nurture productive partnerships, some participants had to be removed from the centers because they were either not sufficiently collaborative or no longer contributed to the direction of the center. Several Managing Directors and PIs said that they did not expect to have to terminate people and found it very difficult. One PI also noted that he felt responsible for helping junior investigators who had been asked to leave, which took time and effort.

We also asked PIs and Managing Directors to describe the characteristics of successful partners and found that there were closely related to the challenges. Respondents indicated that good partners should be invested in the center, committed to working with others toward a common goal, open to different kinds of thinking, and willing to share both successes and failures. The relationship must be seen as a "win-win" for all parties. Several PIs noted that partners should ideally be willing to change course or even abandon their own program to focus on the needs of the centers (as some of them did).

> *"People who are the most effective partners are those who really understand the value of collaborating and are focused on their contribution to a larger project."*
>
> *The successful partners in a Center are ones who change the direction of their research as opposed to doing it on the side."*
>
> *–CCI PIs*

Communication and trust were seen as critical to successful partnerships. One PI said that his center requires attendance at many meetings to keep participants engaged. Consequently, the researchers who were not fully committed to the center left, but those who remained did so for many years. Finally, one PI believed that prior collaboration was helpful to forming successful partnerships.

Center resources allowed CCIs to focus on the most productive research and quickly respond to new scientific developments, but managing resources led to some challenges

One of the strengths of the CCIs mentioned in several PI interviews was their ability to quickly abandon unproductive research directions. PIs indicated that it is not uncommon for investigators on individual grants to stay with a problem because they worry about losing funding if the project fails. In contrast, quick response to scientific developments is encouraged in the CCIs, and is possible because new information is immediately disseminated and resources can be quickly marshalled. To illustrate this point, one PI estimated that it normally takes two years for a new method or idea to be published and another two year to obtain funding to build upon it, while at his centers a response is virtually instantaneous. Finally, PIs indicated that centers can afford to explore uncharted directions that would be too risky or costly for an individual PI to follow. PIs on non-CCI centers included in the study spoke about similar advantages of the center model.

It emerged from interviews with CCI PIs and Managing Directors that internal funding mechanisms they created were instrumental to maintaining center direction and cohesion. They indicated that the requirement that all partners apply for funding every year and the contingency of funding on progress motivates PIs to work toward common goals and be productive. One PI noted that it was helpful to fund projects rather than laboratories, to signal that no one group is entitled to the money. Another established a funding policy that encouraged collaborative publications to maintain center unity, which he found effective. Some of the internal funding strategies developed by CCIs were positively viewed by Site Visitors. For example, they praised seed grant programs available at some centers, especially those supporting the initial exploration of high-risk/high-reward ideas.

However, some challenges related to the allocation of resources also emerged in the study. CCI PIs and Managing Directors reported that the large size of the grant gave some participants the impression that they could get unlimited funding; not funding people at their university led to resentment by some faculty. One PI also mentioned that it was difficult to maintain accountability of partner spending. Several PIs wished that they had included fewer partners in the center (one suggested no more than 11 groups at 8 locations) to reduce management burden on the lead institution and to deepen each partner's involvement. The contention around the distribution of resources brought up by PIs and Managing Directors was echoed by a Co-Investigator, who said that year-to-year uncertainty about the funding made it difficult to support graduate students who work on longer-term projects. Another Co-Investigator thought that the division of funding between partners was not completely fair, although he noted that the process was improving. Finally, we found a small number of comments in Site Visit reports stating that funding allocation seemed arbitrary, lacked transparency, and/or was not linked to grand challenges.

There were advantages to long funding duration

In interviews, some CCI PIs mentioned the advantages of long funding duration (up to 13 years for centers that are successful at all competition stages). They said that given the complexity of the problems and the time it takes for partnerships to gel, it would be impossible to make real progress in less time. PIs also indicated that the long duration of funding to some extent shields the participants from the publish-or-perish academic culture, giving them time to develop new theory and tools to address difficult scientific problems. These advantages were consistent with the results of the CCI investigator survey discussed in detail in our response to RQ 5 in the next chapter.

CCIs had strong leadership

In interviews, Site Visitors, Industry Partners, Co-Investigators, and NSF staff praised CCI PIs for their dedication to the centers, ability to clearly articulate expectations and keep participants engaged, and commitment to transparency and shared governance. One Co-Investigator mentioned their PI's success in bringing Industry Partners to the center and in creating the environment where researchers are not concerned about being "scooped." A Site Visitor told us that PIs were well-respected and trusted, and that he came away from the visit wishing to be a part of this center. Some Site Visitors admired the decisiveness of PIs in removing people who no longer advanced the goals of the center, and one said that he would find this very difficult to do. Interview data were consistent with the survey: 87 percent of CCI investigators were satisfied or highly satisfied with the overall direction of the center, 85 percent with the center leadership, and 86 percent with their experience overall (data not shown).[59]

> *"For the site that I visited, I thought they did an exceptional job. They did a really nice job on their overall management and leadership... They strived to be transparent and open about the decision-making processes which helped all the participants buy in."*
>
> *–CCI Site Visitor*
>
> *"I think the real legacy is in getting everybody on the team to work in a really collaborative environment, which is going to be one of the biggest differentiators between their careers and the people who didn't participate"*
>
> *–Industry Partner*

59 Appendix H, Exhibit H-12, presents complete information for this survey item.

It was also clear from interviews with CCI PIs and Co-Investigators that Managing Directors play an important role in running the center operations. CCI Managing Directors were described to us as a collaborative community of peers, which enables them to share best practices and challenges with each other thus improving all of the centers. Several respondents praised these staff members and wished that the same staff were in the center during Phase I.

In addition to PIs and Managing Directors, the CCI governing structure includes advisory boards, and some comments were made about their composition and utility in administrative records. In general, Site Visitors felt that these bodies were helpful to the centers because they contribute scientific expertise and/or connections to industry. A site visit report for one CCI described the student board at that center as "a phenomenal component" that connected students from all campuses. However, criticisms of the boards were also articulated for some CCIs. Site Visitors thought that some were too limited in expertise (which could lead to "blind spots") or lacked industry representation. In one case, Site Visitors flagged possible conflicts of interest arising from the existing collaborations between the CCI faculty and the advisory board.

> *"Having the Managing Director in there earlier would have been valuable. It would then be the responsibility of that person to build that transition and put the structure in place that uses principles rather than a chemistry professor who has never picked up a book on strategic planning. ."*
>
> *–Managing Director*

CCIs had a collaborative culture

In interviews, several PIs, Managing Directors, and Site Visitors identified collaborative culture as one of the major strengths of the centers. As an illustration, Managing Directors mentioned a shared "playbook," which includes advice on various topics relevant to all CCIs. One Managing Director favorably contrasted his CCI experience with the competitive environment of other centers in which he participated. Internal competition was also mentioned as a challenge by PIs for non-CCI centers. In site visit reports, several centers were praised for a collaborative atmosphere and openness to a range of ideas.

Several CCI PIs and Managing Directors reported that NSF program staff played a key role in promoting this culture. One Managing Director recalled being "plugged into the network" to be quickly trained by peers with more experience. This respondent noted that no one in the CCI community had to learn by themselves and all benefitted from the accumulated knowledge and resources, and consequently the program was improving over time. CCI PIs and Managing Directors also praised NSF for creating a program where each center has the flexibility to develop its own organization and staffing, and for clearly articulating expectations.

> *"I see the other CCIs as my peers, not competition. … It is unique to have the kind of environment where we are rooting for one another and capitalizing on one another's successes."*
>
> *"[NSF staff] has done an outstanding job of creating a network between Managing Directors and directors. It provides a support system that is beyond what most other programs know. And we get continuous feedback and advice."*
>
> *–CCI Managing Directors*
>
> *"The mutual respect for other disciplines and facile collaboration creates a whole that greatly exceeds the sum of its parts."*
>
> *–Site Visit Report*

The NSF staff overseeing the CCI Program was favorably compared to other NSF centers, and many PIs and Managing Directors wished to acknowledge "the enormous role" they played in making their centers successful.

Centers received both positive and constructive feedback on their research programs

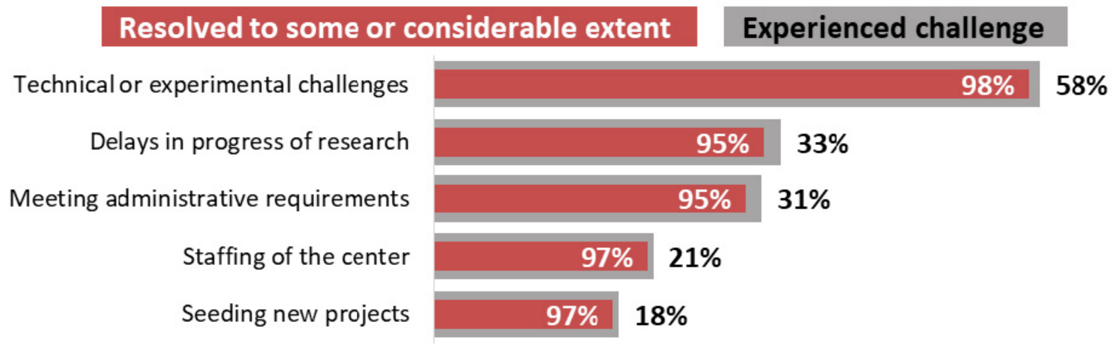
In site visit reports, approximately half of the comments describing the centers' research were positive, and the remaining were either neutral or called for some improvement. On the positive side, Site Visitors highlighted the ambitious vision, high quality of research, and potential for scientific and societal contributions. Some commented that the breadth and/or complexity of the research program was commensurate with the large investment, and praised the intellectual diversity of the team and the "enormous potential" of the work. Other comments were mixed. For example, one panel noted that the center developed powerful new techniques, but lacked vision for how to apply them to advance grand challenges. Another noted that the work had commercial potential, but that the center has not yet articulated any plans for technology transfer. Finally, all CCIs received some negative feedback. For example, one site visit team recommended the establishment of common scientific goals across all partners. Another raised concerns about the potential overlap between CCI and non-CCI grants, and noted that the center did not use the literature to guide their research. A third team felt that the center lacked transformative ideas.

> *"The Site Visit Team felt that [Center] was making important discoveries on numerous projects. The fundamental chemistry will have an important impact in the field, and many of the approaches are novel."*
>
> *"[Center] members have developed an outstanding suite of new techniques that should be used to tackle important chemistry problems. The potential application of these new tools could be large and might encompass many unsolved fundamental questions… However, the center lacks ambitious scientific target questions which may prevent it from making a major contribution to the field."*
>
> *–Site Visit Reports*
>
> *"The level of integration of theoretical and experimental studies is impressive in some research activities, but less effective in others. How to apply existing theoretical tools and/or develop new software tools to address the complex systems [Center] is studying should be actively pursued."*
>
> *–Oversight Memorandum*

Challenges experienced by CCIs were resolved

Survey data revealed that many CCI PIs and Co-Investigators experienced some problems implementing their research program. These included technical or experimental challenges, which were reported by 58 percent of respondents; and delays in progress of research, reported by 33 percent (Exhibit 32). Approximately 20 to 30 percent also indicated challenges in meeting administrative requirements, staffing the center, and seeding new projects. However, nearly all investigators also said that these challenges were resolved (Exhibit 32).

Exhibit 32: Some Investigators Experienced Technical or Organizational Challenges, but These Were Resolved



Note: Q18 N = 134, missing = 0; Q19 N = 79, missing = 0–3.

Source: Survey of Principal Investigators and Co-Investigators Q18 (Has your CCI experienced the following challenges?), Q19 (To what extent have these challenges been resolved?).

Responses for Q18 may not sum to 100% because multiple responses were permitted. Responses for Q19 are limited to respondents who indicated that the challenge had been experienced, according to Q18. Inner bar values are expressed as a percentage of the corresponding outer bar.

Technical challenges reported in the survey were probably related to the publication productivity mentioned in administrative records and interviews. Several Site Visitors believed that per-dollar yield for some CCIs was lower than for individual NSF awards, that contribution among the partners was in some cases uneven, and that some publications reported were only tangentially related to the focus of the center. NSF staff agreed that per-dollar publication productivity of CCIs was lower than for other programs, but noted that this was expected given all of the non-scientific activities of the centers, which took significant resources and time. While explainable, NSF respondents said that low publication yield complicates the task of justifying such large investment to stakeholders. Finally, some Site Visitors criticized CCIs for either not acknowledging the funders or acknowledging multiple funders, which complicated attribution of these results to the CCI grants.

Some CCI PIs and Managing Directors also brought up publication-related challenges in interviews. These included reaching consensus on authorship and content of papers, and identifying journals for interdisciplinary articles. One PI said that the difficult nature of their projects and/or the need to develop a theoretical foundation or instrumentation led to lower-than-normal productivity. Finally, a Managing Director reported that it was difficult to meet NSF's requirement that published papers include co-authors from multiple institutions.

Interviewee concerns about publication productivity were inconsistent with the bibliometric data, which showed that CCI investigators published more papers in better journals than the comparisons, and that these papers were more highly cited (Exhibits 7–10). We speculate on possible reasons for this discrepancy in Chapter 8.

Sub-question 4.2. To what extent and in what ways have the CCIs influenced collaborations among center participants?

Investigators collaborated with numerous partners and expected to maintain these partnerships

Survey data revealed that 58 percent of CCI PIs and Co-Investigators had collaborated with at least one CCI participant prior to the establishment of the center (data not shown),[60] and 98 percent of these investigators said that the nature and/or extent of their collaborations had changed due to CCI participation.[61] Furthermore, these researchers expected to maintain some (71 percent) or most/all (13 percent) of their CCI collaborations after the end of the grant (data not shown).[62] Interestingly, of the respondents who did not get Phase II funding, 76 percent were able to continue working on projects funded through the CCI Program, but this group included only 18 individuals and the results may not be representative (data not shown).[63]

Co-authorship among CCI researchers increased throughout the award

We also examined whether the CCI Program had an effect on collaborations by calculating the frequency of co-authorships before, during, and after participation. Five years before Phase I, 6 to 7 percent of all publications for CCI-affiliated researchers included at least two CCI participants (Exhibit 33). Interestingly, co-authorship among CCI researchers rates were on an upward trend over the pre-CCI period, increasing to 11 to 13 percent.

Once researchers received the CCI award, the co-authorship rate increased sharply, reaching 23 to 27 percent of all publications by the end of Phase I. The patterns for Phase I-only and Phase I/II investigators diverged in the first three years after Phase I ended. For those with a Phase II award, the rates continued to increase, reaching an average of 31 percent by Year 3. In contrast, co-authorship among investigators in centers that were not funded for Phase II awards fell sharply, to 14 percent, returning to the pre-CCI level. Unfortunately, we did not have enough data to examine whether Phase I/II researchers sustain higher co-authorship rates beyond three years and for how long.

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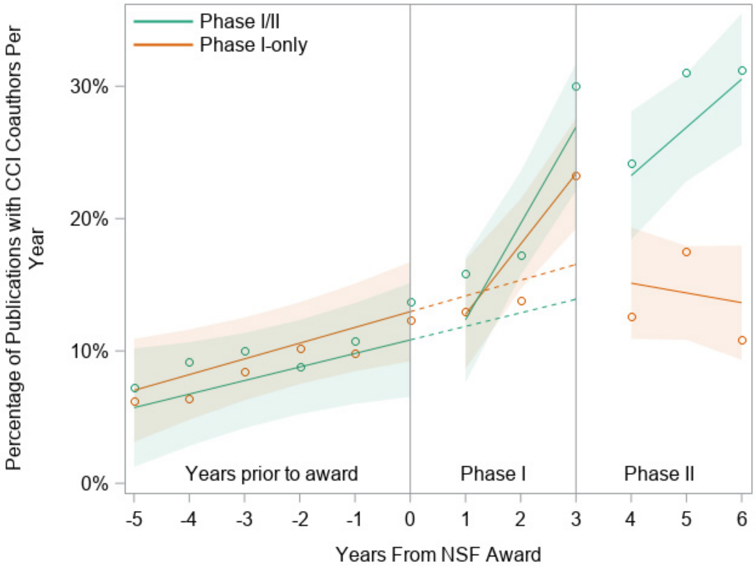
60 Appendix H, Exhibit H-3, presents complete information for this survey item.

61 Appendix H, Exhibit H-4, presents complete information for this survey item.

62 Appendix H, Exhibit H-4a, presents complete information for this survey item.

63 Appendix H, Exhibit H-19, presents complete information for this survey item.

Exhibit 33: Researchers Who Received Phase II Awards Continued to Generate Joint Publications While Those Who Did Not Reverted to the Pre-CCI Co-Authorship Level

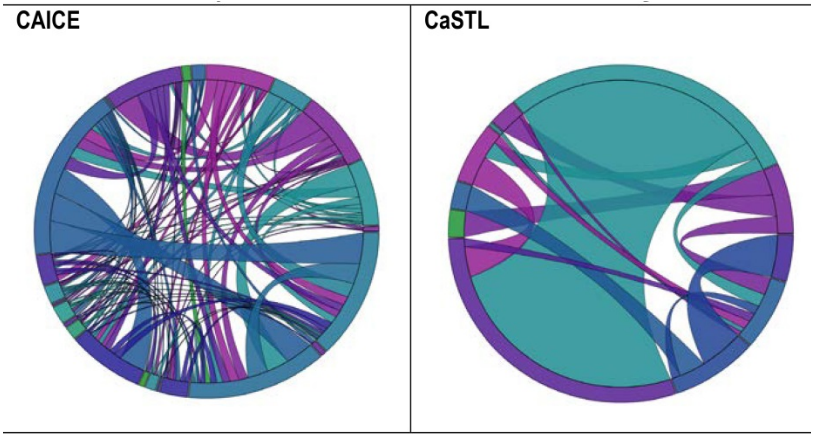


Notes: hollow circles represent average values by group. Solid lines represent linear predicted values, separated by period. Estimated models are interrupted time series, so discontinuities occur at each period boundary. Colored bands represent 95% confidence intervals around predicted values. Dashed lines represent extrapolations of the pre-award period trend into the Phase I period. Prediction models include random slopes and intercepts at the individual level and a first-order autoregressive structure.

Source: all publications in Scopus authored by CCI investigators who participated in Phase I. Investigators in the top one percentile of publications are excluded.

We further explored whether these co-authorships were mainly among a small group of researchers publishing many papers together or many researchers publishing fewer papers with a larger network of collaborators. Exhibit 34 shows two “chord diagrams” that show CAICE having a large numbers of researchers publishing together and CaSTL having fewer researchers publishing together but with larger numbers of publications, including two investigators who co-authored many papers. In these chord diagrams, each colored segment along the perimeter of the circle represents a CCI investigator, and the arcs between two segments represent co-authored publications. The width of the arc is proportional to the number of publications co-authored by two investigators. The variation in size of the perimeter segments indicates whether collaboration within a center is largely driven by a few investigators or more evenly spread among many participants. We found variation in publication patterns across the CCIs – CAICE, CCE, CSN, CCHF, and CSMC involved a high level of collaboration across many participants; Solar, CSP, CaSTL had a few dominant pairings with lower levels of co-authorship from other researchers; and CENTC fell in between. Appendix K includes diagrams for the remaining centers.

Exhibit 34: Example Collaboration Networks with High and Low Density



Source: all publications in Scopus authored by CCI investigators.

Sub-question 4.3. To what extent and in what ways have the CCIs made use of tools and communication to facilitate collaboration?

CCI investigators were satisfied with communications and data-sharing tools, and thought that they contributed to the success of their centers

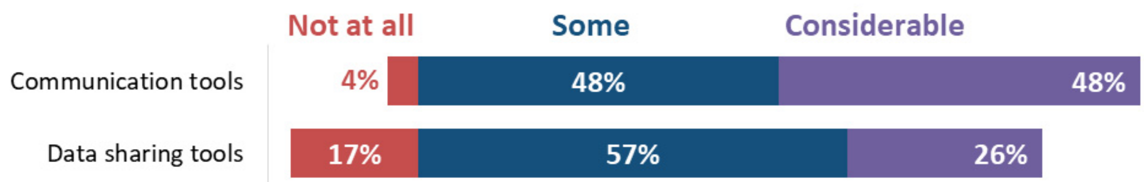
In the survey, 83 percent of CCI PIs and Co-Investigators were satisfied or very satisfied with communications tools, and 67 percent with data-sharing tools (Exhibit 35). Almost all respondents reported that communications and data-sharing tools contributed to the success of their center to some or a considerable extent (Exhibit 36). Respondents at lead institutions were significantly more positive about data-sharing tools than respondents at non-lead institutions ($p < 0.01$, data not shown).

Exhibit 35: The Majority of Participants Are More Satisfied with Communication than Data Sharing Tools Developed by Their CCI

Note: N = 134, missing = 5–22, N/A = 2–36. Three response options (in addition to N/A) are not displayed: "Very Dissatisfied," "Dissatisfied," and "Neutral." To see all the response options, see Appendix H, Exhibit H-12.

Source: Survey of Principal Investigators and Co-Investigators Q15 (How satisfied are you with the following elements of CCI?).

Exhibit 36: The Majority of Participants Reported that Communication and Data Sharing Tools Contributed to Success of Their CCI



Note: N = 85–127, missing = 6–24. Each row is limited to respondents who were not dissatisfied with the element, according to Q15.

Source: Survey of Principal Investigators and Co-Investigators Q16 (To what extent have these elements contributed to the success of your center?).

In the review of center documents, we identified many strategies and tools that were used by CCIs to facilitate communication and data sharing. First, all centers described videoconference-assisted meetings between all or most partners, which were held weekly, bi-monthly, or monthly, depending on the CCI. In addition to center-wide meeting, participants got together in smaller groups of graduate students and postdocs, management teams, or researchers working on the same topic. For example, students and postdocs at one center took turns to give videoconference presentations about their projects to faculty. In addition to these types of virtual meetings, members of several centers met in person two to three times per year.

In addition to videoconferencing, center documents describe many other communication tools. For example, one CCI developed an internal website with a "virtual laboratory," where participants could share ideas and data. Another reported using *Slack* for a similar purpose (this center noted that "this alternative to email reduced the barrier for interested parties to get involved in the conversation"). Other tools described in the reports included *Adobe Connect*, *SeeVogh*, *Google Hangouts*, *GoToMeeting*, *iChat*, *Skype*, *VidYo*, *Webex*, *Access Grid*, electronic notebooks, and *SharePoint*. These platforms were usually restricted to center participants.

We found that some centers were very methodical in developing the best way to interact by piloting various tools and using quantitative feedback from users to make the final choice. Two centers put together tutorials and manuals on how to use the tools they developed, and one wrote a white paper on their communication-related experiences, which was shared with the CCI community. One center used web tools to track collaborative interactions and citations to center publications, and used these data to allocate resources to projects with the greatest impact. Site Visit reports contained many positive comments about data management platforms, which were seen as facilitative of collaboration.

Finally, three CCIs published a newsletter. One of these featured news, events, publications, and announcements. Initially distributed only internally, the center was planning to make it available to its industrial partners and the general public via its website. Another center's newsletter targeted primarily students and postdocs, and was focused on professional development topics. Each edition highlighted the academic journeys and career aspirations of center postdocs.

Chapter 7: Research Question 5 Findings

RQ 5: How effective is the two-phase funding model for the CCI Program?

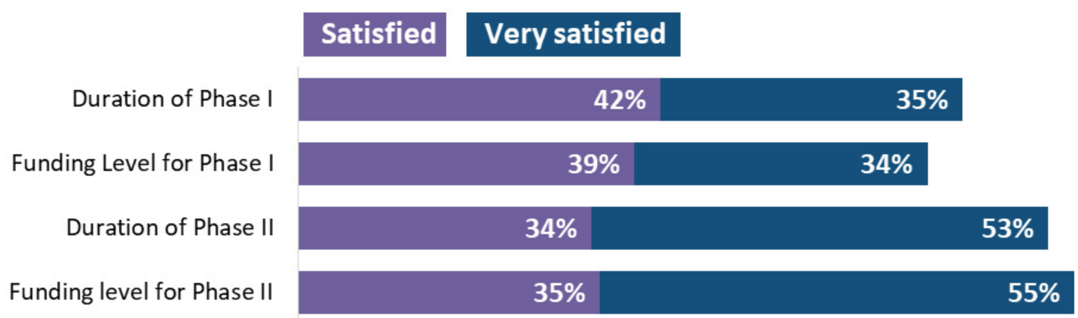
Sub-Question	Extent Addressed	Comment
5.1 What are the strengths and weaknesses of the two-phase award process?	●	Fully addressed in this chapter
5.2 What is the value of the Phase I award experience for the awardees?	●	Fully addressed in this chapter

Sub-questions 5.1 and 5.2. What are the strengths and weaknesses of the two-phase award process? What is the value of the Phase I award experience for the awardees?

CCI Investigators were satisfied with the two-phase funding model

In the survey of CCI PIs and Co-Investigators, we examined satisfaction with the duration and funding level for each phase. We found that these groups were more satisfied with Phase II than Phase I for both funding (90 versus 73 percent) and duration (87 versus 77 percent; Exhibit 37). Nearly all investigators (83 to 94 percent) indicated that both contributed to the success of the center, but funding level and duration for Phase II was again viewed as more important (Exhibit 38).

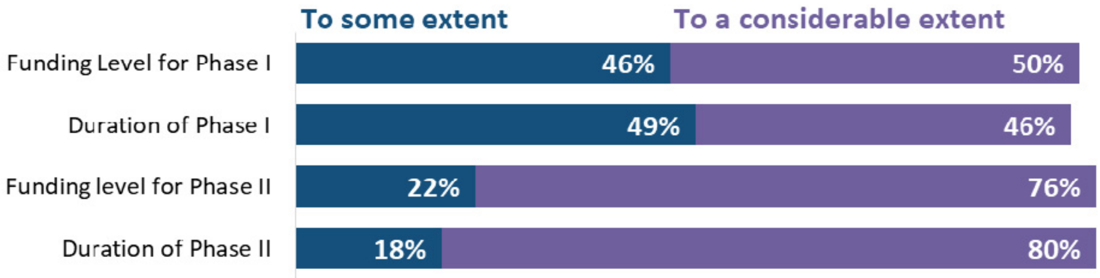
Exhibit 37: CCI Investigators Were More Satisfied with the Funding Level and Duration of Phase II than with Phase I



Note: N = 134, missing = 5–22, N/A = 2–36. Three response options (in addition to N/A) are not displayed: "Very Dissatisfied," "Dissatisfied," and "Neutral." For a table with all response options, see Appendix H, Exhibit H-12.

Source: Survey of Principal Investigators and Co-Investigators Q15 (How satisfied are you with the following elements of CCI?).

Exhibit 38: Funding Level and Duration of Phase II Were More Important to the Success of the Center than Funding Level and Duration of Phase I

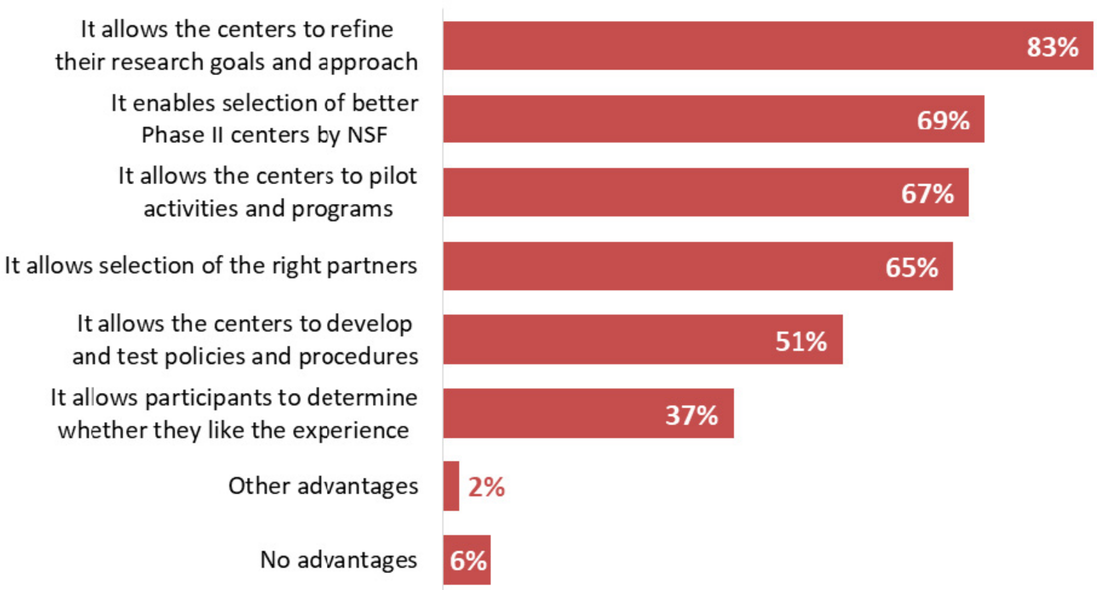


Note: N = 85–127, missing = 6–24. Each row is limited to respondents who were not dissatisfied with the element, according to Q15.

Source: Survey of Principal Investigators and Co-Investigators Q16 (To what extent have these elements contributed to the success of your CCI?).

Many benefits of the two-phase model emerged from the survey. It allowed CCI investigators to refine their research goals and approach (83 percent), pilot activities and programs (67 percent), select the right partners (65 percent), and develop and test center policies and procedures (51 percent; Exhibit 39). About two-thirds of respondents (69 percent) indicated that the funding strategy enabled NSF to select better centers. Ninety-seven percent of CCI PIs and Co-Investigators indicated that participation in Phase I contributed to the success of their Phase II center (data not shown).[64]

Exhibit 39: The Two-Phase Model Allowed Participants and NSF to Select and Build Better Centers



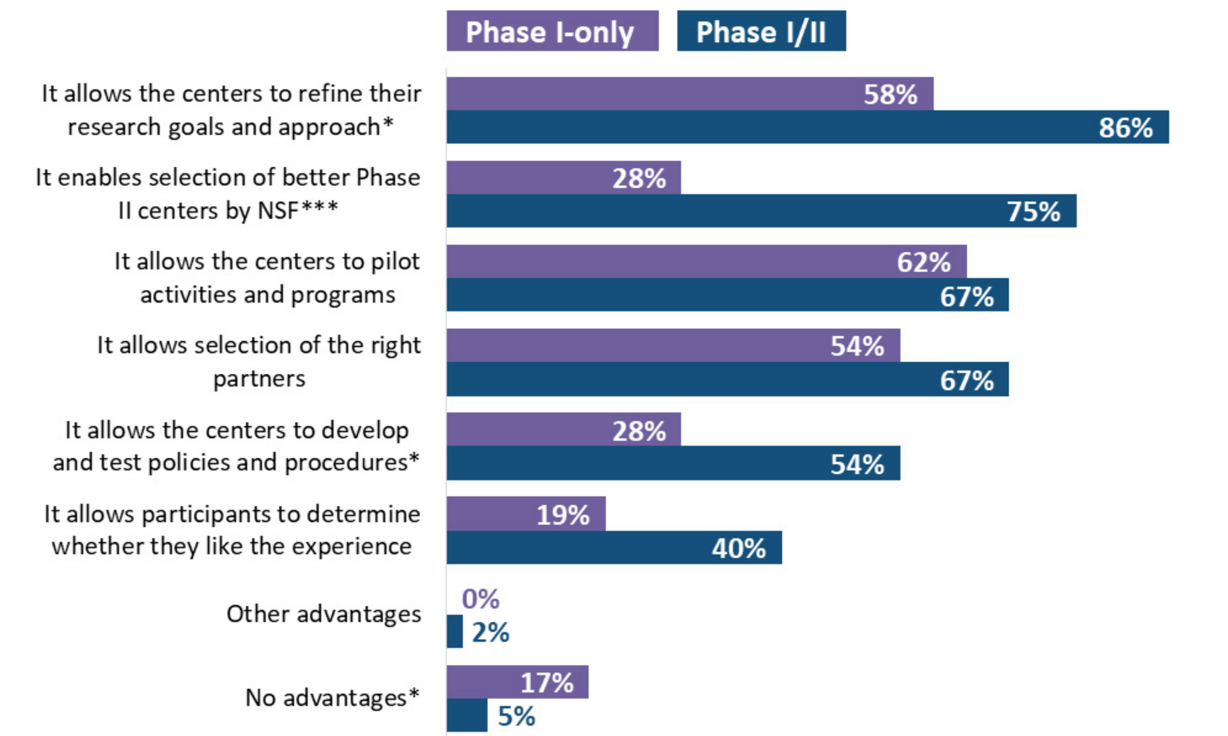
Note: N = 134, missing = 4. Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q23 (In your view, which of the following are the advantages of the two-phase model?).

64 Appendix H, Exhibit H-17, presents complete information for this survey item.

We identified several differences in how grantees who did and did not participate in Phase II perceived the benefits of the two-phase strategy, although we note that the Phase I-only group of the survey respondents included 18 people. Of these, only 28 percent thought that the model enabled NSF to select better centers, compared to 75 percent of the Phase I/II respondents ($p < 0.001$; Exhibit 40). Phase I-only investigators were also much less likely to say that the strategy helps scientists refine their research goals/approach (58 versus 86 percent, $p < 0.05$) and develop/test policies and procedures (28 versus 54 percent, $p < 0.05$). Finally, Phase I-only investigators were more likely to say that there are no advantages to the model (17 versus 5 percent, $p < 0.05$). These differences were not surprising, as Phase I-only researchers have not experienced the second phase and therefore could not appreciate its benefits. It is also possible that their answers were influenced by the disappointment of not having been funded.

Exhibit 40: Phase I-Only and Phase I/II Investigators Differ on their Views of the Two-Phase Model



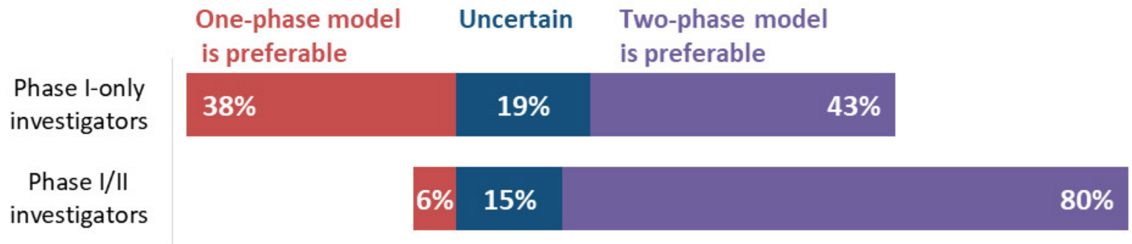
** indicates significance level: * ($p < 0.05$), ** ($p < 0.01$), *** ($p < 0.001$).*

Note: Phase I (N = 18, missing = 2), Phase II (N = 116, missing = 2). Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q23 (In your view, which of the following are the advantages of the two-phase model?).

Consistent with their skepticism about the benefits of this model, 38 percent of Phase I-only investigators preferred a one-phase model, compared to 6 percent of those in Phase I/II (Exhibit 41). However, it is noteworthy that even among Phase I-only respondents, 43 percent preferred a two-phase model.

Exhibit 41: Almost All Phase II Investigators and under Half of Phase I Investigators Prefer a Two-Phase Model

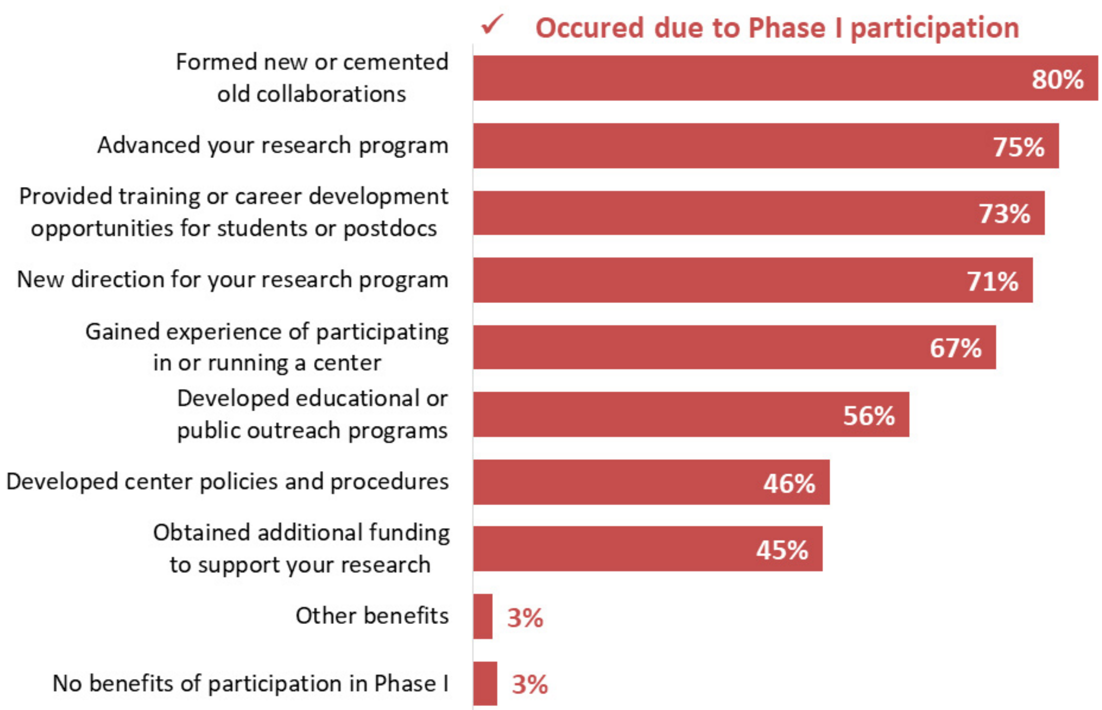


Note: Phase I (N = 18, missing = 3, Phase II (N = 116, missing = 3), responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q25 (On balance, is a two-phase center model preferable to a single phase?).

We also asked Phase II survey respondents to indicate which accomplishments occurred as a result of Phase I. The data were consistent with the benefits of the funding strategy shown in Exhibit 40. Phase I grants enabled participants to establish or cement collaborations (80 percent), advance research program (75 percent), take research in new directions (71 percent), obtain additional funding (45 percent), gain experience participating/running a center (67 percent), train students or postdocs (73 percent), and develop educational or public outreach programs (56 percent; Exhibit 42).

Exhibit 42: Phase I Helped Investigators Form and Sustain Collaborations, Advance their Research, Train Students, Develop Outreach Programs, and Learn How to Run Centers



Note: N = 92, missing = 4. Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q21 (Have any of the following occurred as a result of your participation in Phase I?).

We also discussed both the benefits and limitations of the center-based funding strategy in general, and of the two-phase model specifically in interviews, and virtually all respondents endorsed the two-phase model. Several CCI PIs and Managing Directors reported that it would be very difficult to launch a center of their size and complexity without preparation (some called it "unimaginable"); even with Phase I, the centers had to go through "growing pains" when they transitioned to Phase II. All CCI respondents, except one who had experience with other centers, said that the CCI model was preferable, and some recommended that NSF adopt this model for all center programs. The single dissenting CCI Co-Investigator had a positive experience with MRSEC and STC programs, suggesting to him that Phase I was unnecessary. This respondent expressed concerns that some researchers who would likely be successful in Phase II had been excluded after putting much effort into establishing their center. He argued that while NSF might view the two-phase mechanism as a strategy to mitigate risk, it was unreasonable to "pull the rug out" from Phase I researchers.

"Phase I centers allows the core team to get formulated, so that they can start working out what their research goals are and come into the Phase II with a clear vision of what the center looks like, scientifically and personally. It gives more time to build a logical team."

–CCI Managing Director

"You can be a really, really good chemist and not be a good leader. The initial phase screens out the people who are not going to be able to hold together a very large funding mechanism. I actually think that's quite important."

–CCI Site Visitor

"Maybe in some fields you can jump into the center, but it would have been very hard to do for this one."

–CCI PI

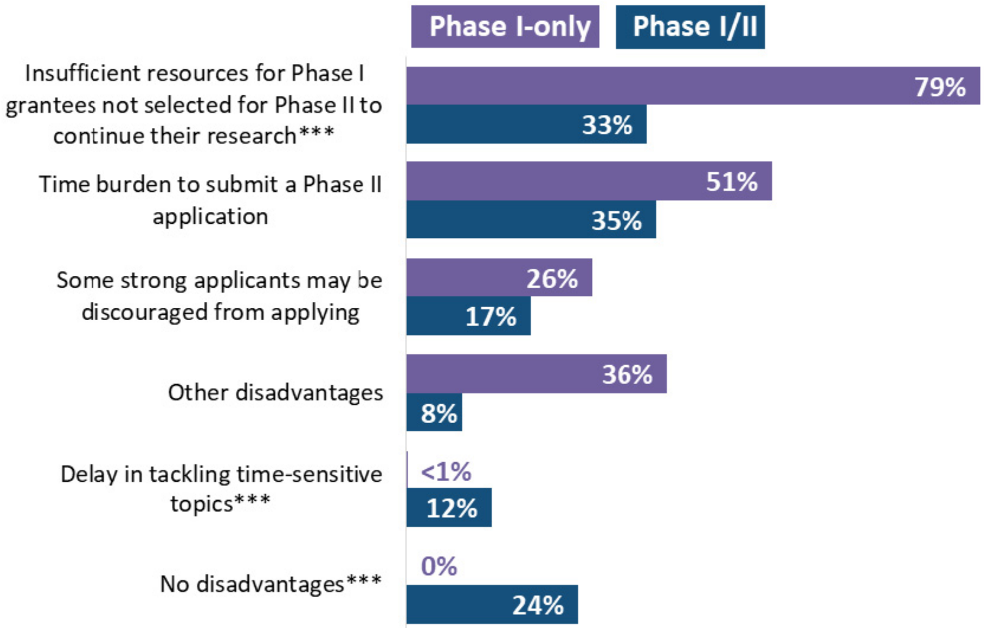
Interview respondents identified several specific benefits of the first phase, which were consistent with the survey data. According to CCI PIs, Phase I is necessary to develop the center mission, determine how various experts fit together to address this mission, plan the center structure and polices, and write a realistic proposal for a larger center. Some PIs also commented that the Phase I grant helps participants determine whether this mode of research appeals to them and that the competition for the Phase II grant motivates participants to develop a better center. Consequently, the first phase mitigates risk for NSF by directing larger investment to the centers with the strongest scientific mission and teams. NSF staff echoed this last point. They indicated that more centers fail because of "human failings than science." Finally, NSF staff argued that the Phase I grant is valuable in and of itself as it offers researchers an opportunity to work on higher-risk and/or larger projects.

A few respondents commented on the size of Phase I awards. NSF staff said that while the funding level is relatively low, it is adequate for putting the infrastructure and teams in place and that a center should not be given a larger grant if it cannot accomplish this goal. NSF staff and one PI also argued that the small size of planning grants helps select people who are committed to the concept.

A few disadvantages of the two-phase model also emerged

In the survey, 79 percent of Phase I-only investigators and 33 percent of Phase I/II indicated that the model provides insufficient resources to Phase I grantees not selected for Phase II to continue their research ($p < 0.001$; Exhibit 43). About one-fourth of Phase I-only investigators (26 percent) indicated that some strong applicants may be discouraged from applying for CCI funding knowing that they would have to compete again for a Phase II award. Thirty-six percent of Phase I-only investigators selected the "other" option for the question about disadvantages, and entered explanatory comments. Several respondents wrote that the funding amount was insufficient to meet the requirements for Phase II, favoring pre-existing teams. Others noted opportunity costs incurred by those who had invested their time in a Phase I project, but could not sustain the project without Phase II funding. One Phase I-only investigator suggested that NSF provide some support for unsuccessful Phase I centers that had established promising collaborations.

Exhibit 43: Disadvantages of the Two-Phase Model Include Insufficient Resources to Continue the Research and Time Lost in Submitting an Application for Phase I-Only Centers



** indicates significance level: * (p < 0.05), ** (p < 0.01), *** (p < 0.001).*

Note: Phase I (N = 18, missing = 2), Phase II (N = 116, missing = 2), overall (N = 134, missing = 4). Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q24 (In your view, what are the disadvantages of the two-phase model?).

Several limitations of the two-phase model were also mentioned in interviews with respondents not participating in CCIs. One non-CCI center PI said that this type of program may not create "the same level of excitement" in the community, and that the burden of writing additional proposals and reports may not add value. One Site Visitor expressed concern that the time to put together a competitive Phase II proposal delays the actual work of the center. Another Site Visitor thought that it was too onerous to put so much effort into organizing a center, while facing relatively low odds of being awarded the larger grant. In place of Phase I, he suggested requiring applicants to demonstrate that they can develop a successful center in proposals or early on after the award is made. This respondent also noted that center grants are often written by assistant professors, who benefit little, especially if the Phase II is not funded. Finally, a Site Visitor said that he was uncomfortable with the instruction from NSF that a Phase II center had to be "worth the full $20 million or they get nothing." Several CCI PIs agreed that not all problems required such large investment and that NSF should also fund smaller centers if it is appropriate for their proposed research program.

NSF staff also identified several drawbacks of the model, which included the burden on the agency and the community to review Phase I proposals, the risk of excluding strong Phase I centers, and the effects on Phase I investigators who had "invested their heart and soul for three years" on not being selected for Phase II. Like survey respondents, some interviewees suggested that NSF sets aside some funding to support promising Phase I projects that did not make the cut for Phase II.

CCI PIs and Managing Directors identified three challenges. The first was that Phase I centers lacked the resources to hire Managing Directors. They argued that not only this makes preparing for Phase II more difficult, but it also commits these staff to activities and programs into which they had no input. Another challenge was related to the much larger size of Phase II. PIs and Managing Directors reported that they had to recruit many new members who were not part of Phase I and may not understand the center culture, mission, and policies. Finally, one CCI Co-Investigator noted that successful Phase II centers should have an option to continue beyond 10 years, although he acknowledged that this may be not be feasible.

Chapter 8: Conclusions and Recommendations

We conducted a mixed-methods evaluation of the NSF CCI Program, which was launched in 2004. The sample included 14 centers that received only Phase I awards and 9 centers that received Phase I and Phase II awards funded through 2017.

The evaluation aimed to address five research questions and 14 sub-questions posed by NSF, was informed by a literature review, and was approved by the external TWG and by NSF evaluation and CCI Program staff. The study drew on a review of CCI annual reports, proposals, and websites; site visit reports; funding/oversight memoranda; internal interim reviews and review analyses; interviews with NSF staff, Site Visitors, CCI PIs, Managing Directors, Industry Partners, Co-Investigators, and PIs on non-CCI center grants; surveys of CCI PIs, Co-Investigators, students, and postdocs; and analysis of publications authored by CCI investigators and PIs on individual NSF grants. These data were triangulated to the extent possible to address the RQs. In this chapter, we offer our conclusions and recommendations by Research Question.

Research Question 1: What are the important contributions of the CCI Program to our current understanding of fundamental chemistry?

What is the evidence of productivity and influence of the scientific research?

The analysis of full publication records of CCI and non-CCI investigators and of the subset of papers that acknowledged CCI funding suggest that the program had a positive effect on productivity. Prior to joining the centers, CCI investigators had publication rates that were similar to those of the comparison group, but by the end of Phase I their productivity was significantly higher, at 12 versus 8 papers per year ($p < 0.01$). Furthermore, investigators participating in Phase II continued publishing at this rate over the next three years, while the productivity of Phase I-only and comparison groups declined. Finally, the papers of all CCI participants regardless of the phase received significantly more citations than those of the comparison PIs.

An analysis of 2,054 CCI-acknowledging papers enabled us to examine the benefits of Phase II and revealed that it significantly improved center-level publication productivity. Three years after the end of Phase I, Phase II centers published 26 CCI-acknowledging papers per year across investigators, while this number for Phase I-only centers declined to 0. Finally, CCI participants published in journals with significantly higher impact factors than a random sample of comparison investigator publications ($p < 0.001$) and Phase II researchers outperformed Phase I-only on this measure ($p < 0.05$).

While it seems likely from the data that CCI participation had at least contributed to these positive outcomes, we cannot rule out the effect of confounding variables (for example, CCI participants could be more senior and/or better funded than the comparisons). However, survey data produced additional and more direct, albeit self-reported, evidence to support the benefit of CCI funding. Nearly two-thirds of responding investigators (65 percent) reported an increase in productivity and 43 percent in journal quality following CCI participation.

Numerous examples of specific advances were cited in the administrative documents and interviews, but we were unable to determine to what extent these accomplishments made advances toward addressing grand challenges in fundamental chemistry and how they impacted the field due to their highly technical nature. We compiled the accomplishment profiles for each Phase II center by culling these documents that could be evaluated by experts.

To what extent and in what ways have the CCI centers demonstrated leadership in their field and in what ways has the chemistry research community benefited from the CCI centers?

The study provided strong evidence that the program offered many benefits to researchers affiliated with the centers. Nearly all CCI PIs and Co-Investigators reported being able to recruit better students and postdocs, obtain additional funding, broaden research program, and more rapidly respond to scientific developments. These CCI participants also reported improvements in professional visibility and recognition, and one Site Visitor said that CCI PIs became "household names." Survey respondents also believed that CCI funding benefited the broader research community as CCI-developed methods, educational and outreach materials, communication infrastructure, data, reagents, and equipment are used outside of the centers. Finally, many respondents highlighted the contribution of CCIs to developing well-rounded young scientists and educating the public about science.

We were able to validate some of these views using other sources of data. First, journal impact factor and citation data showed that articles acknowledging CCI funding are published in high-impact journals and presumably influence other scientists. Second, we gathered significant data from students and postdocs, which demonstrated the positive role of CCIs in training the next generation of scientists, benefiting the scientific community at large.

> ***Recommendation: Use an independent expert panel to further evaluate the scientific contributions of CCIs and their influence of the research community.*** While we were able to capture the scientific output of CCIs through bibliometric analysis and by culling proposals and annual reports, NSF could consider engaging experts in CCI fields to further understand the nature and importance of their scientific advances. It is probably worthwhile to delay this review by a few years, so that the influence of CCI work could be more clearly determined.

Research Question 2: How successful have the CCI centers been at transferring their basic research results into societal or economic benefits (innovation)?

In annual reports, most CCIs described traditional indicators of commercialization, such as industry partnerships, inventions, licenses, and patents. Eight of the nine centers also launched companies to develop degradable plastics, energy storage devices, a polymer platform, and instrumentation to assess atmospheric aerosols. In the survey, CCI PI and Co-Investigators reported benefits to industry resulting from the centers that included reduced environmental impacts, cost savings, and increases in the sales of products. However, none of the four industry partners interviewed confirmed these benefits. Without comparison groups or benchmarks, we are uncertain how to evaluate CCI performance in the area of commercialization. Given the relatively recent establishment of the program and its focus on basic chemistry, the commercial output is probably reasonable. We also note that it is probably too early to expect many societal or economic benefits of CCIs, which are in any case are difficult to both measure and attribute.

A potentially more significant impact of CCIs on commercialization is through workforce development, which we were able to document. In the surveys, approximately one-third of graduate students and one-quarter of postdocs said that a position in industry became their career goal after joining a CCI; just under one-third of investigators also reported an increased interest in commercialization. Industry partners confirmed the contribution of CCIs to bringing together the academic and industry communities, and in training students and exposing them to this sector.

Research Question 3: What are the contributions of the CCI Program in the areas of workforce development (education and professional development), broadening participation, and informal science communication?

What are the most important impacts of CCIs in these three areas and how was this made possible (or enhanced) by the center mechanism of operation?

Workforce development

According to the survey of PIs and Co-Investigators, CCIs launched or improved numerous professional opportunities for students and postdocs. These included not only disciplinary training through courses, seminars, and research experiences, but also the development of transferrable skills, such as communication, leadership, mentoring, and management. Many graduate students and postdocs had multiple mentors and opportunities to present at CCI meetings and to visit partner laboratories, broadening their horizons and helping them to develop connections. CCI investigators believed that these activities, which were made possible by the center, improved the quality of education in chemistry and made these researchers more competitive on the job market. Site Visitors praised CCIs for their programs and commented on the excellent research skills of students and on their maturity.

CCI graduate students and postdocs who responded to the survey confirmed that they had access to a broad range of opportunities and most were satisfied or very satisfied with their experiences. Approximately three-fourths (76 percent) reported a collaboration with researchers outside of their institution and one-quarter worked at a partner's laboratory. The vast majority of graduate students and postdocs also reported that participating in CCI was advantageous to their careers, because they were exposed to a broad range of scientific areas and had better access to faculty, peers, equipment, facilities, and reagents. Consequently, they felt well-prepared to conduct research, work in teams, think critically, solve problems, communicate, and mentor. However, the survey also revealed that less than 50 percent applied for grants and fellowships, visited other research labs, taught, and were involved in entrepreneurship. At the same time, fewer than 30 percent indicated that they were well prepared to teach, write proposals, and work outside of academia – the very same skills these activities would enhance.

Finally, some graduate students and postdocs reported that the CCI experience had influenced their choices of institution, discipline, and research problem, and had improved access to job opportunities. Of the 220 researchers who had left CCIs, 44 percent had a position at a college or university, 29 percent in industry, and 12 percent in government. In summary, the available data provided strong evidence that CCIs played a positive role in the career development of junior scholars.

Broadening participation

In the survey and in administrative records, CCI participants described many programs and activities to recruit and retain URGs. These included visits to schools, opportunities for K-12 and college students to conduct research at CCI universities, and even a girls' science television show. CCI staff attended conferences sponsored by professional societies to learn about strategies to broaden participation, and to recruit and retain students. They also partnered with HBCUs and other educational institutions to bring faculty and students to CCIs. Once recruited, the centers made efforts to on-board and mentor minority students by pairing them with peers. In the survey, most CCI investigators indicated that these activities had increased the diversity of their laboratories and institutions and nearly all that the diversity programs had contributed to the success of their centers.

Examination of the demographic characteristics of the CCI graduate students and postdocs revealed that the centers were comparable to the national average in the representation of women (36 percent at CCIs versus 38 percent nationally), and performed better in the representation of racial/ethnic minorities (14 percent versus 9 percent). However, these statistics may not accurately describe the composition of the centers as only about half of the CCI graduate students and postdocs completed the survey.

The comments in site visit reports were mixed. While Site Visitors acknowledged CCI efforts to broaden participation, they also noted that some centers lacked clear goals and implementation plans, and should try to increase diversity among the faculty.

Informal science communication

Data collected in the survey, review of documents, and key informant interviews revealed that all CCIs engaged in public outreach. Virtually all PIs and Co-Investigators believed that these activities helped educate the public and contributed to the success of the centers. Program documents listed numerous examples of activities for people of all ages offered at a broad range of venues. Many of the programs targeted K-12 students to encourage them to enter STEM fields.

In interviews and annual reports, the centers offered evidence that some of their products reached large audiences. For example, an educational video about chemical bonds had been incorporated into the curricula at 80 schools and 3,000 high school students from all over the world are searching for new materials as part of the "Solar Army" program. Industry Partners and Site Visitors saw public outreach as an important component of the centers, although they also recommended assessing these programs for effectiveness. One Co-Investigator noted that NSF should provide clearer guidance about the expectations for the scope of outreach and for the definition of progress.

The study provided sufficient evidence to conclude that CCIs created numerous innovative and unique outreach programs, and at least some of these are engaging the public. However, we do not have the data to judge the success of these efforts.

To what extent and in what ways have the CCIs contributed to sustained, institutionalized change in these three broader impact areas?

The majority of CCI PIs and Co-Investigators indicated in the survey that various programs and partnerships for workforce development, broadening participation, and public outreach were sustainable. However, interviews with CCI staff, NSF program managers, and Site Visitors indicated that the legacies of CCIs will include collaborations, scientific contributions, best practices for running a large center, companies based on CCI technologies, educational materials, and scientists trained at the center. We suspect that the opinions expressed in interviews are more realistic, but do not have the data to support this view.

> ***Recommendation: Encourage CCIs to offer more opportunities for junior scholars to teach, apply for funding, participate in entrepreneurship, and work in partner organizations.*** While we acknowledge the breadth and scope of CCI programs in workforce development, the survey revealed that less than 50 percent of graduate students and postdocs participated in these particular activities. At the same time, these researchers reported lacking some of the skills these opportunities would develop. Centers might consider creating these types of activities if they do not already exist or encouraging their students to take advantage of them.

Research Question 4: How effective are the center structures and operations in achieving the program's goals?

Leadership and culture

In interviews, all or nearly all Site Visitors, Co-Investigators, and NSF staff praised CCI PIs for their personal dedication to the centers, ability to articulate expectations, commitment to transparency and shared governance, and team management skills. Managing Directors also emerged as playing an important role in running the center operations and by disseminating effective strategies and challenges across the centers; two Managing Directors noted that it would be very valuable to have this position in Phase I. In general, CCIs were consistently described in interviews as having a very collaborative culture, which was characterized as unusual by some of those who had experience with other centers. Consistently, the analysis of publications by CCI investigators showed a dramatic increase in the level of co-authorships during the grant, from 6–7 percent to 23–27 percent. Several PIs and Managing Directors credited NSF staff with creating and maintaining this environment, and with the resulting success of the CCIs.

Publication productivity

Several Site Visitors believed that publication rates for CCIs were lower than for individual NSF grants per dollar invested and that some reported publications were only tangentially related to the focus of the center. A few NSF staff also said that the publication productivity of CCIs was lower than for other programs, but thought it was reasonable given the complexity of the problems and the investment in non-scientific programs. Finally, some CCI PIs and Managing Directors also brought up lower productivity, which they attributed to challenges in finding journals that would accept interdisciplinary papers, the need to reach consensus among multiple senior authors, and the need for theoretical or methodological foundational work that is not necessarily publishable.

Interestingly, these views were not borne out in the bibliometric analysis, which showed that CCI PIs published more papers per year, on average, than PIs on individual NSF grants. Several possibilities may explain this discrepancy. Bibliometric data reflected per-person rather than per-dollar productivity, and in interviews, respondents may have been referring to the expected productivity for such a large center rather than for individuals. In addition, the publication dataset includes high outliers, which makes the entire CCI community look more productive and masks less-productive investigators. In contrast, interview subjects and site visit reports may have focused on individual researchers or centers with relatively low productivity.

Partnerships

In the survey of PIs and Co-Investigators, the majority of CCI researchers were satisfied with the contributions of their partners, communication tools, frequency and productivity of meetings, and distribution of resources. Retention in the centers was high, with 95 percent of investigators affiliated for two years or longer and 54 percent for seven years or longer.

Survey data revealed that 58 percent of CCI PIs and Co-Investigators had collaborated with at least one CCI participant prior to the establishment of the center, and 98 percent of these said that the nature and/or extent of their collaborations had changed due to CCI participation. The vast majority of collaborating researchers expected to maintain at least some of these relationships after the end of the grant. Interestingly, three-quarters of Phase I-only investigators continued working on CCI projects, but this sample was small (n = 18) and may have been biased toward people who are more likely have continued their CCI research. Nonetheless, some of the collaborations are persisting.

We also used the bibliometric analysis to examine partnerships. The analysis of publications by CCI investigators showed a dramatic increase in the level of co-authorships during the grant, from 6–7 percent to 23–27 percent. The rate increased to 31 percent for the researchers participating in Phase II, but returned to the pre-CCIs levels for the researchers not participating in the second phase. At some CCIs, co-authorship rates were driven by a small number of researchers who published frequently, while in others, the networks included many center members co-publishing at lower rates.

Several challenges related to partnerships emerged from the study. The most frequently reported, both in the survey and in interviews, was terminating partnerships that were unproductive or no longer aligned with the goals of the center. CCI PIs and Managing Directors indicated that they had not expected to have to remove people from the center and found it very difficult. PIs also said that the hardest part of running the center was integrating participants with diverse interests and expertise into a cohesive research program, and maintaining their focus on the mission of the center. From the experience directing CCIs, PIs came to appreciate the importance of carefully assessing the true capability of each partner, setting goals that are clear and interesting to everyone, articulating expectations, and maintaining frequent communication. PIs indicated that the best partners were willing to subordinate their own research program to the needs of the center.

Resource allocation

One of the strengths of the CCIs mentioned in PI interviews is their flexibility – both in abandoning unproductive directions and in rapidly marshaling resources and expertise to respond to new developments. CCIs also have the “luxury” to explore scientific problems that a single PI would consider too risky or costly. Similar advantages of the center model were mentioned by PIs on non-CCI centers.

Internal funding mechanisms created by CCIs were instrumental to maintaining center direction and flexibility. PIs mentioned several strategies they found effective, which included annual funding allocation contingent on progress to motivate participants, funding projects rather than laboratories to signal that no one group is entitled to resources, and favoring projects that have resulted in collaborative publications. Site Visitors remarked positively on some of these mechanisms, such as seed grants for high-risk/high-reward projects.

However, some challenges related to the allocation of resources were also articulated in interviews and in the survey. PIs and Managing Directors mentioned difficulties in monitoring partner spending and animosity from some faculty at their university who had not been funded. The contention around the distribution of resources was echoed by Co-Investigators, who said that year-to-year funding uncertainty made it difficult to support graduate students and that the division of funding between partners was not completely fair. A small number of comments made by Site Visitors in administrative records also indicated that the allocation of resources seemed arbitrary, lacked transparency, and/or was not linked to grand challenges.

> ***Recommendation 1: Continue with the center funding mechanism.*** We collected strong evidence from multiple sources revealing the benefits of this mechanism to scientific research, visibility and reputation of faculty, professional development of students and postdocs, and the promotion of public understanding of science.

> ***Recommendation 2: Consider providing optional funding for a Managing Director position in Phase I or other creative solutions to project management.*** It clearly emerged from the study that these staff play an important role in the centers. Having this support available in Phase I would allow PIs to focus on the scientific mission and partnerships of the larger center.

Research Question 5: How effective is the two-phase funding model for the CCI Program?

The CCI funding strategy was strongly endorsed by researchers who participated in both Phase I and Phase II. Survey respondents said that the first phase allowed them to refine their research goals and approach, pilot activities and programs, select the right partners and cement partnerships, develop and test center policies and procedures, take research in a new direction, obtain additional funding, and train students and postdocs. About two-thirds of CCI PIs and Co-Investigators indicated that NSF was able to select better centers by using this mechanism, and nearly all who were involved in Phase II centers said that their participation in Phase I contributed to the success of their center. Survey respondents also expressed satisfaction with the duration and the funding level of each phase. Perhaps not surprisingly, researchers whose centers had not been selected for Phase II awards were much less likely to indicate these benefits of a two-phase model. It is noteworthy, however, that even among this group, slightly more still preferred two phases to one.

A few limitations of the model also emerged. One of these was the opportunity cost and potentially wasted efforts of unsuccessful Phase I PIs, which was mentioned by CCI PIs both participating and not participating in Phase II centers, Site Visitors, and NSF staff. Approximately one-quarter of CCI investigators and a PI from a non-CCI center also expressed a concern that some potentially strong applicants may not wish to participate in the program because of the two-phase format. A Site Visitor and CCI PIs also identified a lack of flexibility in the size of Phase II award as a limitation, noting that not all centers require such a large investment. Finally, about one-third of Phase I/II PIs, one-half of Phase I-only PIs, and at least one Site Visitor indicated that the time required to submit a Phase II proposal was a potential weakness of the mechanism because it took time away from research.

> ***Recommendation: Continue with the two-phase funding strategy.*** The two-phase approach was strongly endorsed by most participating researchers, particularly those that were awarded Phase II awards.

Summary of Findings

In summary, this evaluation has yielded substantial information about the operation and outcomes of the CCI Program. We found that the majority of researchers at all career levels were very satisfied with their experiences and explicitly linked their time at CCIs to many important professional outcomes. Program participants were also in agreement about the advantages of the center model in general and the two-phase mechanism specifically, and endorsed this funding strategy for future centers. The CCI community produced a large body of published work and launched numerous programs to support workforce development, public education, and participation of racial/ethnic minorities and women in STEM. While the evaluation was non-experimental in design and relied heavily on self-reported data, the breadth and consistency of evidence collected from multiple sources allows us to conclude that the CCI Program is meeting its intended goals.

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Two-Phased Approach to Funding

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Appendix A: Literature Review

To inform the evaluation design and data collections/analysis strategies, we conducted a review of publications, agency reports, evaluation reports, national surveys, funding opportunity announcements, and CCI Program documents. The review focused on several broad topics embedded in the research questions, which included:

- Productivity and influence of scientific research
- Societal or economic benefits of research
- Broader impacts
- Research centers
- Two-phased research

In this appendix, we summarize the information that emerged from the review. Following, we present an evaluation framework with a list of indicators which were used in previous studies or developed by our team based on our experience and the literature. This appendix also includes the references used for each broad topic and the grand challenges in chemistry and those faced by society, as identified by various organizations.

A.1 Productivity and Influence of Scientific Research

Research Impact/Influence

Productivity is a measure of efficiency and is generally determined by the ratio of outputs to inputs (www.epa.gov/evaluate/program-evaluation-and-performance-measurement-epa). In the context of scientific research, productivity is associated with generating and disseminating new knowledge. The most common measures of productivity for an individual researcher or research unit are the total number of publications (Inside Consulting and Oxford Research, 2005; Lee and Bozeman, 2005; Lin and Bozeman, 2006; Chubin et al., 2010; Environment Canada, 2014; Schneider et al., 2014; Waltman, 2016) and patents (Wagner & Alexander, 2013; Schneider et al., 2014; Waltman, 2016). Publication lists are easily available from publicly available and commercial databases, such as PubMed, Web of Science, and Scopus.

Some scholars relied on outputs other than journal articles to measure knowledge dissemination. These include books and book chapters, conference proceedings, seminars, workshops, and research conferences (Inside Consulting and Oxford Research, 2005; Chubin et al., 2010; Schneider et al., 2014; Gibson & Daim, 2016; Waltman, 2016). Data for these indicators are typically self-reported by scientists in surveys (Inside Consulting and Oxford Research, 2005; Chubin et al., 2010; Schneider et al., 2014) and/or abstracted from databases such publication databases mentioned above.

As indicators of productivity, these bibliometric measures have many desirable characteristics: they are scientifically-derived, easily understood, scalable, accessible, and relatively low-cost to obtain (NRC, 2012). At the same time, they do not capture the full breadth of activities vital to a fully functioning scientific production system (Schmoch, 2009; Inside Consulting and Oxford Research, 2005). Other important indicators of research productivity reported in the literature include:

- *Training of students* – the total number who participated in research and the number of graduates (Schmoch & Schubert 2009; Wagner & Alexander 2013)
- *Research infrastructure maintenance* – participation in the peer review process (Schmoch & Schubert 2009; Schmoch et al., 2010)
- *Technology and knowledge transfer* – consultation or collaboration with industry and participation on scientific advisory boards with cross-sector membership
- *Commercialization* – creation of new research tools, methodologies, and databases (Schmoch & Schubert 2009; Wagner &Alexander 2013).

Furthermore, contribution of any research program should be considered in terms of impact or influence of the products it generates on the scientific community (www.epa.gov/evaluate/program-evaluation-and-performance-measurement-epa). Research impact is frequently measured through citations to publications, including their total number, average number per publication, number/proportion of highly cited papers, citation percentiles normalized for publication year, and citation networks (Inside Consulting and Oxford Research, 2005; NRC, 2007; Bornmann et al., 2013; Schneider et al., 2014; Waltman, 2016).

Other citation-based indicators include journal impact factors and the h-index. While also frequently used (Chubin et al., 2010; Costas et al., 2010; Schneider et al., 2014), these indicators can be misleading (Corneliussen, 2016; Kreiner, 2016). For example, journal impact factor gives disproportionate significance to a few very highly cited papers (and a high level of citation can be the unintended result of an artifact, such as an article error). Furthermore, citations and any indicators derived from them only capture the impact of journal publications, effectively leaving out other types of outputs. However, this limitation is less significant for chemists, who tend to disseminate knowledge via journal articles, and which have excellent coverage in the Web of Science and Scopus databases (Moed, 2007).

Finally, other indicators of scientific impact and research quality which emerged from the literature are formal recognition by the community through awards, prizes, appointments to editorial boards of prestigious journals, and invitations to speak at important conferences (Chubin et al., 2010; NRC, 2007; MRC 2013/14 Report) as well as success in obtaining funding for research (Chubin et al., 2010; Langfeldt, 2010; Lal et al., 2011; MRC 2013/14 Report). This type of data is usually collected directly from researchers in surveys, interviews, or review of resumes, personal websites, and biosketches.

Scientific Leadership and Responsiveness

Our review of the literature revealed that scientific leadership is generally equated with high publication productivity and/or other measures of impact or recognition described in the previous section (Klavans & Boyack, 2010; Environment Canada, 2014; NRC, 2007; Schneider et al., 2014; Waltman, 2016; Clarivate Analytics, 2016). However, Klavans and Boyack (2008) also proposed another type of leadership, referred to as “thought leadership,” which compares the reference age of the citations used by a research unit to an average reference age for that field. These authors argued that the research which builds on more recently cited literature may be more innovative.

Scientific responsiveness can be defined as a research unit’s ability to anticipate, adapt to, and respond to new science realities and priorities (Environment Canada 2014). In fact, the 2017 NSF CCI solicitation (17-564) indicates that a CCI center should be “agile structures that can respond rapidly to emerging opportunities.” Given these definitions, responsiveness and leadership are closely related concepts.

Important to a research unit's ability to adapt and be agile is their ability to maintain the broad expertise and capacity needed for new science realities and priorities (Environment Canada, 2014). Some evidence of this linkage exists. Ponomariov and Boardman (2010) indicate that including participants and stakeholders from divergent contexts, backgrounds, and sectors (i.e., government, academia, and industry) in a research unit can help build the necessary scientific capacity for addressing complex scientific questions. Greater diversity also increases the overall network of the research unit, which can be tapped into for changing scientific realities (Environment Canada, 2014).

Innovative and Transformative Research and Outcomes

A primary objective of CCI is to fund innovative and potentially transformative research. The NSF defines transformative research as "ideas, discoveries, or tools that radically change our understanding of an important existing scientific or engineering concept or educational practice or leads to the creation of a new paradigm or field of science, engineering, or education. Such research challenges current understanding or provides pathways to new frontiers" (https://www.nsf.gov/about/transformative_research/definition.jsp).

Several other terms are often interchangeably used in the literature with transformative research. For example, "breakthrough" research "challenges existing theories and scientific paradigms," applies "radically new ways of using methods," and relies on "unprejudiced combination and interdisciplinary integration of different research perspectives" and is also characterized by an "exceptional risk of failure" (Hayrynen, 2007). High risk/high reward, creative, innovative, and pioneering are also common (Heinze and Bauer, 2007; National Science Board, 2007; Lal et al., 2011). However, innovation typically implies a demonstrated use that has been put into practice with measurable social and/or economic benefits (described in detail below).

While the term transformative research has been better defined in recent years, no agreed upon measure has emerged (Lal et al., 2011; Schneider et al., 2014). Some studies postulated a link between transformative research and research productivity and/or impact, and used these well-accepted indicators as proxies (Heinze and Bauer, 2007; Lal et al., 2011; Wagner and Alexander, 2013; Tinkle et al., 2016). Beyond typical bibliometric analysis, Schneider et al. (2014) proposed a novel citation analysis method to identify "breakthrough" papers by using extremely highly cited papers in combination with additional filtering and network analysis to remove noise and establish far-reaching impact. This method was tested to evaluate the extent that grants funded by the Danish Council for Independent Research produced "breakthrough" research compared to other funding programs. Finally, some authors postulated that transformative research necessitates interdisciplinary approaches and/or the use of unproven equipment, techniques, or methodologies (Lal et al., 2011) and therefore could be operationalized through these characteristics.

Expert judgement is often used to determine whether research is transformative. In this approach, experts are asked to rate a set of projects funded under traditional and transformative/innovative programs on a set of characteristics, which include novelty, risk, and innovativeness, and the ratings are compared. This types of studies were conducted to evaluate the UK's Wellcome Trust programs, the NIH Pioneer and New Innovator programs, and the NSF's INSPIRE program (Grant et al., 1999; Lal et al., 2011; Tinkle et al., 2016; Bobronnikov et al., 2016). Alternatively (or in addition), researchers themselves are asked to render judgement on the transformative nature of their work and/or to compare the research they conduct under traditional and innovative funding mechanisms (Wagner and Alexander, 2013; Kolarz et al., 2016; Bobronnikov 2016; Chubin et al., 2010; Lal et al., 2011).

We note that some scholars suggested that long-term funding is a key element to promoting transformative research, as it provides researching the time and resources necessary to experiment, fail, and adapt (Laudel et al., 2014).

Grand Challenges in Chemistry

In recent decades, the concept of "grand challenges" has been used by foundations, funding agencies, professional societies, and other groups to articulate fundamental, intractable problems faced by society. These are problems that require coordinated and sustained effort as well as extensive resources to solve, but if solved, could have significant, far-reaching impact (George, 2016). Some grand challenges target broader societal problems, such as the United Nation's Sustainable Development Goals (United Nations, 2015), while others focus on particular intractable problems faced by a specific group or field of study. The purpose of a grand challenge is to foster innovation by clearly identifying the problem and mobilizing expertise and resources to approach it (Ofir, 2016). Solutions to grand challenges are expected to be unconventional, requiring diverse expertise, out-of-the-box thinking, and new methods and techniques – in other words, have the characteristics of potentially transformative research.

In Appendix B we provide several lists of grand challenges in chemistry: by the authors of a National Research Council report released in 2006 (NRC, 2006), by the editors of Scientific American in 2011 (Ball, 2011), and by the editors of American Chemical Society Central Science in 2016 (Bertozzi et al., 2016), as well as lists of societal grand challenges by the European Union Horizon 2020 (European Union Horizon) and the United Nation's Sustainable Development Goals (United Nations, 2015).

A.2 Economic Benefits of Research

Definitions and Measures of Innovation and Economic Development

Research is thought to drive innovation and economic development. Broadly defined, innovation is the development of a new or significantly improved product or process (NASEM, 2017a). Outputs of innovation are embodied in goods and services and then exchanged in the commercial marketplace (Stone & Lane, 2011; NASEM, 2017a). The creation and diffusion of new technologies, products, and ideas in the commercial marketplace have the potential to generate social, health, and economic benefits to particular groups (Stone & Lane, 2011; Lane & Flagg, 2010). Research competitiveness is the ability to take new knowledge, apply it to industrial use, attract firms and capital investment and use it to build economic clusters that strengthen the regional economy (Atkinson & Nager, 2014; Porter, 2003; Sum & Jessop, 2013). Economic development is the process through which an economy grows or restructures to become more advanced, especially when both economic and social conditions of a community are improved (Cambridge Dictionary, 2018).

Scholars suggest several approaches to measuring the social and economic benefits that stem from research results. One is to capture an organization's commercial contributions (NASEM, 2017a), such as invention disclosures, licenses, patent applications, patents, start-up companies, and manufactured products. Some studies also used applications to the programs which support research commercialization, such as Grant Opportunities for Academic Liaison with Industry (GOALI) and Small Business Innovation Research (SBIR)/Small Business Technology Transfer (STTR).

Surveys are typically the primary method for collecting data on the societal and economic benefits of research and innovation. However, because of low response rates and increasing costs, more researchers are turning to analysis of administrative created for operational or reporting purposes (NASEM, 2017a). The key advantage of relying on extant data is that it is not subject to desirability bias (Hall, et al., 2012).

Engaging with Partners in Commercialization

Technology transfer is defined as the dissemination of new products, processes, or intellectual capital across organizational boundaries, which then leads to improvements in processes or productivity (Nagle, 2007). The types of partners engaging in technology transfer vary in number and the extent to which they collaborate (Smilor et al., 2007; Trauth et al., 2015). Government-industry-university partnerships are thought to be the ideal model because of the cross-fertilization of ideas that arise when different actors form social connections that are beneficial to knowledge sharing (Trauth et al., 2015). Anticipated benefits of these partnerships, in addition to commercialization, include networking, career, and professional opportunities (McGowen, 2017).

We identified several indicators for assessing the formation and development of partnerships that engage in technology transfer. One set of indicators include the number and types of partners involved (Smilor et al., 2007; NASEM, 2017a). Other indicators are focused on the interaction between universities and industries, including engaging through technology transfer offices, experiential programs for students, hiring of students by industry, and alignment of research and industry needs (Owen-Smith & Powell, 2001; Trauth et al., 2015; NASEM, 2017a; Lane et al., 2014; Grimaldi et al., 2011; Nagle, 2007). Some authors traced the careers of students and researchers to industry and government to investigate how training and research experience can build cutting-edge skills and knowledge across sectors (Lane et al., 2014). Other indicators that measure partnerships are the culture of collaboration, the intent to sustain the partnership, the geographic proximity of knowledge transfer, and the percent of industry funding (Trauth et al., 2015; Perkmann et al, 2011; McGowan, 2017; Bostrom, 2010; Ponds et al, 2010; Franklin, 2009).

A.3 Broader Impacts

As described by NSF, "broader impacts may be accomplished through the research itself, through the activities that are directly related to specific research projects, or through activities that are supported by, but are complementary to, the project" (CCI Solicitation 17-564). For CCI, the focus of broader impacts are in four areas: a) promoting the translation of transfer of the basic research results into societal or economic benefit; b) promoting workforce development through educational and professional development training activities; c) increasing diversity and broadening the participation of underrepresented groups in chemistry; and d) communicating research to public audiences via informal science. Since the translation of research into societal or research benefit are covered above, in this section we focus on the other three broader impacts.

Promoting Workforce Development

Broadly, workforce development includes the activities, policies, and programs that provide individuals with opportunities for sustained work and help organizations achieve goals within a societal context (Haralson, 2010; Jacobs & Hawley, 2009). Literature focusing on the development of students in the STEM fields has highlighted a range of activities, for which participation can be measured, that help achieve these individual and organizational goals. One set of workforce activities help individuals envision themselves in a professional role, and can be measured by participation in mentoring, research opportunities, and internships. STEM mentors have been positively linked to career decisions and the pursuit of STEM careers (Dorsen, Carlson, & Goodyear, 2006). Research opportunities enable students to be socialized into the sciences (Hunter, Laursen, & Seymour, 2007; Piper & Krehbiel, 2015;

Seymour, Hunter, Laursen, & DeAntoni, 2004), and can also serve as mentoring experiences (Packard, 2012). Likewise, internships can provide hands-on training, while also helping to recruit future workers and integrate them into the workplace faster (Olson & Riordan, 2012; Symonds, Schwartz, & Ferguson, 2011). Individuals who participate in these activities have also been found to express higher rates of job satisfaction (Olson & Riordan, 2012).

Another related set of workforce indicators focus on creating a nurturing environment at the institutional level to ensure that individuals feel connected to the intellectual and social aspects of an organization (Piper & Krehbiel, 2015). Some literature has also highlighted the potential for near-peer mentoring with, for example, graduate or other upper-level students providing mentorship and building a community (Olson & Riordan, 2012). Other activities to promote a positive climate include regular contact with program staff, social gatherings with peers and staff, seminars, courses, and support networks (Piper & Krehbiel, 2015; Rodriguez & Anderson-Rowland, 2013).

Finally, STEM workforce development also includes a set of indicators designed to measure students' experiences in professional activities that foster professional success, such as publishing, developing courses or training materials, teaching, and presenting at conferences. Research indicates, for example, that publication and collaboration with faculty and advisors as graduate students predicts career success and productivity (Pinheiro, Melkers, & Youtie, 2014). Further, the development of educational materials and/or teaching not only provides hands-on preparation for the future, but the process of teaching may also improve research skills when combined with a research experience (Feldon et al., 2011). Opportunities to attend conferences allow students to improve presentations skills (Gardner & Barnes, 2007), foster an increase in professional confidence and identity (Seymour et al., 2004), and interact with a professional community in their field (Seymour et al., 2004).

Increasing Diversity and Broadening Participation of Underrepresented Groups

NSF has a long history of investing in strategies aimed at increasing participation of underrepresented groups in STEM (James & Singer, 2016). In particular, investments have focused on two broad strategies: 1) integrating education and research to develop a diverse STEM workforce and 2) building a highly skilled, diverse workforce by investing in recruitment, training, leadership, and management of talented individuals (NSF, 2014). Measuring the success of these goals can be accomplished using a range of indicators at the individual and institutional level (Bensimon, 2004; Garcia et al., 2001; Smith, Parker, Clayton-Pedersen, Moreno, & Teraguchi, 2006). At the individual level, measures of the recruitment and retention of underrepresented groups (URGs) provide indicators of access at institutions and a metric of how institutions foster success (Bensimon, 2004; Clewell & Fortenberry, 2009; Garcia et al., 2001; Smith et al., 2006; Whittaker & Montgomery, 2014). Also at the student level, individual experiences are measured to better understand the experiences that URGs are having, and whether these experiences are those that will enable future success (Clewell & Fortenberry, 2009; Garcia et al., 2001; Smith et al., 2006).

Several institutional level metrics provide an indication of structural transformation aimed at equity and inclusion of URGs. These range from a plan for diversity that demonstrate an institution's commitment to broadening participation of URGs (Clewell & Fortenberry, 2009) to policies and practices, such as mentoring (Bensimon, 2004; Garcia et al., 2001; Smith et al., 2006; Stassun, Burger, & Lange, 2010; Whittaker & Montgomery, 2014), and the creation of campus diversity committees (Smith et al., 2006). A number of authors have also noted the importance of collaborations and partnerships that leverage Historically Black Colleges and Universities (HBCUs)/Minority Institutions (MIs), and other organizations focused on diversity (Clewell & Fortenberry, 2009; Stassun et al., 2010; Whittaker & Montgomery, 2012; Williams et al., 2011).

Informal Communication of Research to Public Audiences

Science communication is “the exchange of information and viewpoints about science to achieve a goal or objective such as fostering greater understanding of science and scientific methods or gaining greater insight into diverse public views and concerns about the science related to a contentious issue” (NASEM, 2017b). Communicating scientific research to the broader community is widely believed to be an important responsibility of scientists (Dewey, 1927; Greenwood & Riordan, 2001). Previous research has highlighted the efficacy of disseminating to the community via informal channels, leveraging the idea that everyday experiences can reach all people (National Research Council, 2009). To that end, previous research has highlighted several sets of informal experiences that can be used to engage the public (Council, 2009), and measurement of the extent to which scientific institutions participate in these activities can be used to assess the extent to which dissemination goals are being achieved.

One set of informal activities centers around spaces that support science learnings, including museums, science and environmental centers, zoos, and aquariums (National Research Council, 2009; Nisbet & Markowitz, 2016). These spaces engage participants in a way that showcases science’s relation to real world phenomena, and allow them to pursue and reflect on science interests (National Research Council, 2009). Another set of informal activities are more structured and take place in schools and community based organizations (National Research Council, 2009). Although these activities target a motivated group of individuals who have elected to participate in these activities, research suggests that they can positively affect academic achievement and students’ career orientation (National Research Council, 2009). Furthermore, research suggests that scientists also benefit from participation in these activities, as they can use them as opportunities to improve communication skills (Clark et al., 2016). A third set of activities center around outreach, including participation in community events, public presentations, demonstrations, science cafés, and other similar events (Brownell, Price, & Steinman, 2013; NASEM, 2017b).

A final set of informal activities involves dissemination through the media, including the radio, television, internet, and other electronic platforms (NASEM, 2016, 2017b; National Research Council, 2009; Pavlov et al., 2018). Evidence exists to suggest that dissemination of science via educational television impacts science learning, but the effectiveness of dissemination through other platforms is less clear (National Research Council, 2009). Not surprisingly, the younger the individual, the more likely they are to consume information about science and technology through the internet, online newspapers and magazines or other electronic platforms (NASEM, 2017b).

Leadership in Broader Impacts

In the NSF’s *Perspectives on Broader Impacts* (15-008), the authors discuss that collaboration between NSF, institutes of higher education, nonprofits, and other partners can mitigate some of the challenges associated with achieving broader impacts. For example, collaborations between chemists and experts in science communication can strengthen both parties through reciprocal exchange of expertise; furthermore, these collaborations can help support a community of practice for implementing effective strategies on a larger scale (NASEM, 2016). Collaborations with historically black colleges and universities (HBCUs), minority serving institutions (MSIs), and/or organizations with expertise supporting groups underrepresented in STEM both help enrich the academic community and meet the mentorship and other needs of minority students (NSF CREST and HBCU-RISE solicitation 18-509; Chubin et al., 2017). Finally, connecting educational and employment organizations within and across sectors can strengthen the accountability systems and help form career pathways for participants at all stages (Chubin et al., 2017; Harkavy et al., 2017).

In addition to effective collaborations, NSF also recommends consideration of leadership's commitment to broader impact efforts and the use of existing institutional resources (e.g., human, infrastructure, instruments, and fiscal) as well as new and creative elements for providing high quality broader impact activities (NSF 15-008). For example, the NSF Centers of Research Excellence in Science and Technology (CREST) and HBCU Research Infrastructure for Science and Engineering (RISE) (18-509) are expected to provide leadership in the involvement of groups traditionally underrepresented in STEM at all levels (faculty, students, and postdoctoral researchers) within the center, and centers are required to use either proven or innovative mechanisms to address issues such as recruitment, retention and mentorship of participants from underrepresented groups.

The National Alliance for Broader Impacts (NABI) offers leadership guidance in broader impacts, whether groups are building on existing activities, programs, or infrastructure or developing new ones (NABI, 2016). They describe the importance of considering whether new elements need to be introduced to the existing infrastructure; how the proposed activity would transform an existing program or how a new program would transform knowledge, processes, and models for the intended audience; whether the activity leverages other resources; what other partners or collaborators are important to implement the activity; and what is the value added.

A.4 Research Centers

Federal agencies, for-profit companies, universities, and foundations are investing in scientific collaborations that span disciplines and institutions in order to bring together scientists with differing expertise and perspectives to solve pressing scientific problems (Hall et al., 2008; Vogel et al., 2012). These efforts resulted in growing body of knowledge on center operations and the role of center mechanism in promoting discovery.

Effective Center Management Strategies

Several scholars argued that research centers, in particularly those linking scholars from different disciplines, pose both participation and leadership challenges. These include communicating administrative matters across the center, coming to consensus on the team's goals, and meeting the requirements and needs of respective institutions (Glied et al., 2007; Wong-Parodi & Strauss, 2014).

We found that centers identified a range of management strategies to facilitate productive collaboration. For example, some employed a site coordinator and found this position highly effective for facilitating communication and resolving administrative and management issues (Sonnenwald, 2004). Review of the literature also revealed the importance of stakeholder and partner involvement in center governance. For example, one study found that centers with governing boards containing only local members reported more strained relationships than those with more diverse bodies (Langfeldt et al., 2010). Another center created stakeholder advisory boards so that industry, government, and non-profit representatives could access center resources and forge relationships with faculty, and found this practice to be useful (Ponomariov et al., 2010). A review of a European network found that over 80 percent of participating organizations developed a shared action plan with their partners to use as a guiding tool. Other popular collaborative activities among network participants included the creation of shared proposal procedures and research agendas and, to a lesser extent, of cooperative agreements between participating entities (Doussineau, 2014).

Some centers adopted policies to improve support for faculty and students. These included changes to tenure policies to reward collaborative work and team science (Guise et al., 2017). We also found evidence that centers actively expose young scientists to broad, interdisciplinary topics and offer opportunities to cultivate the social skills needed to collaborate. For example, undergraduate or graduate students are placed in interdisciplinary forums, required to interface with multiple mentors, and taught to synthesize information from multiple viewpoints (Guise et al., 2017).

Finally, research centers have developed a variety of tools and strategies to facilitate collaboration and streamline communication processes. These include various types of meetings, which may be large or small and in-person or virtual. Centers also create written documents to clearly articulate goals, career development plans, and mentorship expectations. For example, one center reported using formal and informal assessments of mentor-mentee relationships as a tool to facilitate coordination and collaboration (Ponomariov et al., 2010; Guise et al., 2017). Interestingly, respondents in one study reported that certain tools, such as joint calls, were burdensome and did not contribute to the cohesiveness or coordination of research team (Doussineau, 2014).

Role of Center Mechanism in Advancing Research

We identified several papers that discussed how to assess whether center collaboration have led to more impactful research (Hall et al., 2008; Vogel et al., 2012; Wuchty et al., 2007; Lee & Bozeman, 2015; Ponomariov et al., 2010). For example, Wuchty suggested that interdisciplinary collaboration was associated with more publications and higher numbers of citations to these publications (Wuchty et al., 2007). This idea received support in the study by Ponomariov, who concluded that affiliation with a center improved productivity and enabled interdisciplinary and inter-institutional collaboration (Ponomariov et al., 2010). Some studies examined changes in co-authorships and funding success among faculty participating in research centers (Ponomariov et al., 2010; Chubin, 2010; Hall, 2008).

In addition to bibliometric indicators, other tools are used to assess center performance. These include conducting surveys of center participants to examine whether and to what extent the programs are achieving their goals. Finally, some evaluators rely on in-depth qualitative interviews to better understand the impact on research collaborations and the career trajectories of participants (Doussineau, 2014; Hall et al., 2008).

A.5 Two-Phased Approach to Funding

Kolarz et al. (2016) argued that transformative research is inherently uncertain, and therefore risky. Consequently, funding agencies and industry look for approaches to mitigate these risks. A two-phase approach, where funding for the second phase is contingent on some demonstration of progress in the first phase, is one such strategy. We found that this type of strategy has been used in software development industry, where fast pace requires constant innovation and creativity (Napier et al., 2008).

A two-phase strategy is also used for the Small Business Innovation Research/ Small Business Technology Transfer (SBIR/STTR) program funded by the federal government. As with other programs, the goal of the Phase I award is to demonstrate the technical feasibility of the proposed innovation (often by developing a prototype), which is followed by a competitive and larger Phase II award to commercialize the invention. For this program, as with other multi-phase programs, the research and development undertaken in Phase I is intended to have a high level of risk, so it is expected that not all projects will achieve their desired technical outcomes. Projects that are successful are in a better position to obtain follow-on funding. The Phase I minimizes the risk in later phases of the work.

The CCI Program also uses a two-phase funding model to minimize funding risk and put the structures in place for a successful Phase II Center. The goal of Phase I, with a budget of up to $600 thousand per year for three years, is to develop the management and teaming structures of the centers and to engage in research, broader impact activities, and center development activities. The research may build on pre-existing activities, but new, collaborative results are expected. The Phase I awards provide researchers the opportunity to pilot and develop center-scale activities (CCI solicitation 17-564).

Projects that receive the two phases of funding from the CCI Program receive a minimum of eight years of funding with the potential for additional follow-up funding. This long-term funding has been identified as a key element to promoting transformative research as it provides researching the time and resources necessary to experiment, fail, and adapt (Laudel & Gläser, 2014).

While the two-phase approach to funding is clearly used across programs to minimize risk, we have not come across any studies which examined its effectiveness.

Appendix B: Evaluation Framework

This appendix has two parts. First, we present the full set of indicators developed by the study team during the evaluation initiation phase based on the review of the literature and our own experience with evaluations of research programs.[65] The indicators are presented for each research question and referenced; for each indicator we list the data sources, the analytic approach, and any comparison groups used, organized as tables. In the second part of the appendix, we include a fuller description of how each data source referred to in the tables was originally planned to be used.

B.1 Mapping of Research Questions to Indicators, Analytic Approaches, and Comparison Groups

Research Question 1: (Modified): What are the important contributions of the CCI Program to our current understanding of fundamental chemistry?

(Original: What are the impacts of the CCI Program on our current understanding of fundamental chemistry?)

1.1 (Modified) What is the evidence of productivity and influence of the scientific research?
(Original: What is the evidence of productivity and impact of the scientific research?)

Research Productivity

1. Publications (Chubin et al., 2010; NRC 2007; Schneider et al., 2014; Costas et al., 2010)
2. Books/book chapters (Chubin et al., 2010; Inside Consulting and Oxford Research, 2005; Schneider et al., 2014)
3. Conference papers (Schneider et al., 2014; Waltman, 2016)
4. Patents (Inside Consulting and Oxford Research, 2005; Schneider et al., 2014; Cooperative Research Center Evaluation; MRC 2013/14 Report; Wagner & Alexander, 2013; SIR methodology)
5. New knowledge developed through research (Abt developed)
6. Research conferences, workshops, seminars (Chubin et al., 2010; Inside Consulting and Oxford Research, 2005; Gibson & Daim, 2016)
7. Students trained, degrees received (Schmoch & Schubert, 2009; Wagner & Alexander, 2013; Gibson & Daim, 2016)
8. Scientific advisory board participation, policy advice, testimony (Schmoch and Schubert 2009)
9. Receipt of awards, fellowships, or chaired positions (TWG suggested)
10. New research tools created (Wagner & Alexander, 2013; Gibson and Daim, 2016)
11. New methodologies created (Wagner & Alexander, 2013; Gibson and Daim, 2016)
12. Databases created (Wagner & Alexander, 2013)
13. Internal perspective on research productivity (Abt developed)
14. External perspective on research productivity of CCIs (Abt developed)

[65] While the study team was not able to collect data on each of these indicators, the set of indicators informed the design and data collection for the study.

Indicators	Data Source	Analytic Approach	Comparison Group
1-3	Publications from Phase I and II annual reports; Scopus database	Descriptive statistics for CCI and comparison publications	PIs on individual grants in chemistry
4	Patents and patent applications from Phase I and USPTO database	Descriptive statistics for patent applications and awards	None
5-11	Open-ended data in internal and external Phase II program documents	Abstraction and coding of all relevant information; selected examples to include in Center profiles	None
12	Survey of PIs/Co-Investigators, item 10; interviews with PIs	Descriptive statistics for survey items	PIs on center grants (interviews)
13	Open-ended data in external Phase II program documents; interviews with individuals involved in oversight of CCIs	Abstraction of all relevant information; summary of external comments	None

Research Impact and Collaboration

1. Citations, including number of "hot" papers and citations in patents (Schneider et al., 2014; Waltman, 2016; NRC 2007; Costas et al., 2010; Salimi, 2017; Bornmann et al., 2013; Clarivate Analytics; SIR Methodology)
2. Journal impact factors (Schneider et al., 2014; Costas et al., 2010)
3. Collaboration network based on co-authorship (Keserci et al., 2017)
4. National and international, cross-disciplinary, and trans-sector collaborations (Schmoch et al., 2009; Salimi, 2017; MRC 2013/14)
5. Awards, prizes, and accomplishments (Chubin et al., 2010; NRC 2007; MRC 2013/14 Report)
6. Speaking invitations (NRC 2007; MRC 2013/14 Report)
7. Follow-up funding (Chubin et al., 2010; The Research Council of Norway, 2010; MRC 2013/14 Report; Gibson & Daim, 2016)
8. Service on editorial boards, review panels, advisory boards (Schmoch & Schubert, 2009; Schmoch et al., 2010)
9. Description of impact by grantees (Abt developed)
10. External perspective on research impact (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1-4	Publications from Phase I and II annual reports, Scopus database	Analysis of citations to CCI and comparison publications; analysis of publication-based network; analysis of publication authorships	PIs on individual and center grants in chemistry
5-8	Open-ended data in internal and external Phase II program documents	Abstraction and coding of all relevant information; selected examples to include in Center profiles	None
9	Survey of PIs/Co-Investigators, item 10; interviews with PIs	Descriptive statistics for survey items	PIs on center grants (interviews)
10	Open-ended data in external Phase II program documents; interviews with individuals involved in oversight of CCIs	Abstraction of all relevant information; summary of external comments	None

1.2 To what extent and in what ways have the CCI centers demonstrated both leadership in their field and responsiveness to developments in their field?

Scientific Leadership

1. High performer based on publication productivity (Klavans & Boyack 2010; Environment Canada 2014; NRC 2007)
2. High performer based on number/proportion of highly cited papers (Klavans & Boyack 2010; NRC 2007; SIR Methodology; Schneider et al., 2014; Environment Canada, 2014; Waltman 2016; Clarivate Analytics)
3. Notable awards and honors (Chubin et al., 2010; NRC 2007; MRC 2013/14)
4. Conducting potentially transformative/innovative/breakthrough research (Chubin et al., 2010; Wagner et al., 2013; Grant et al., 1999; Bobronnikov et al., 2016)
5. External perspective on scientific leadership (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1-2	Publications from Phase I and II annual reports, Scopus database	Analysis of citations to CCI and comparison publications	PIs on individual grants in chemistry
3	Open-ended data in internal and external Phase II program documents	Abstraction of all relevant information; coding of selected examples to include in Center profiles	None
4	Survey of CCI Phase I and II PIs and Co-Investigators, item 5	Analysis of ratings of project characteristics linked to transformative research	Benchmark against Abt INSPIRE survey
5	Open-ended data in external Phase II program documents; interviews with individuals involved in oversight of CCIs	Abstraction of all relevant information; summary of external comments	None

Scientific Responsiveness

1. Research addresses grand challenges (Environment Canada, 2014)
2. Research unit has ability to adapt to new science realities or priorities (Environment Canada, 2014)
3. External perspective on responsiveness to developments (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1	Open-ended data in Phase II internal and external Phase II program documents	Mapping of grantee research to known grand challenges	None
2	Survey of CCI Phase I and II PIs and Co-Investigators, item 9	Analysis of ratings of survey data on group agility	None
3	Open-ended data in external Phase II program documents	Abstraction of all relevant information; summary of external comments	None

1.3 Does the center mechanism of operation contribute to the research achievements of the centers?

Changes due to CCI participation:

1. Publication productivity (Branco, 2010; Chubin, 2010; Hall, 2008; Ponomariov et al., 2010)
2. Journal fields, number of co-authors, affiliation of co-authors (Wuchty et al., 2007; Ponomariov et al., 2010)
3. Changes in publication patterns, visibility/reputation (Abt developed)
4. Use of new instrumentation, technology, data, approaches, increased diversity of research problems (Abt developed)
5. Access to additional resources, such as staff, equipment, facilities, funding (Abt developed)
6. Role of center mechanism in changes (Branco, 2010; Chubin, 2010; Hall, 2008; Ponomariov et al., 2010)
7. External perspective on the role of center mechanism (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1-2	Publications from Phase I and II annual reports, Scopus database	Analysis of publication and authorship data	PIs on individual grants in chemistry
3-6	Survey of CCI Phase I and II PIs and Co-Investigators, items 9 and 10; interviews with Phase II PIs/Co-Investigators	Analysis of ratings for survey data; summary of themes emerging from interviews	PIs on center grants (interview data)
7	Open-ended data in external Phase II program documents	Abstraction of all relevant information; summary of external comments	None

1.4 (Modified) In what ways has the chemistry research community benefited from the CCI centers? *(Original Question: To what extent and in what ways has the chemistry research community benefited from the CCI centers?)*

Ways in which CCIs may benefit the chemistry research community:

1. Resources and infrastructure created or improved by CCI, such as methods, communication infrastructure, facilities, lessons learned for how to run a center (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1	Open-ended data in Phase II program documents; survey of CCI Phase I and II PIs and Co-Investigators, item 11; interviews with CCI Phase II PIs and Co-Investigators; interviews with industry partners, and individuals involved in oversight of CCIs	Abstraction and coding of all relevant information; selected examples to include in Center profiles; descriptive statistics for survey items; summary of themes emerging from interviews	

Research Question 2: How successful have the CCI centers been at transferring their basic research results into societal or economic benefits (innovation)?

2.1 (Modified) In what ways have the research findings and other center achievements contributed to societal and economic benefits? *(Original Question: To what extent and in what ways have the research findings and other center achievements contributed to societal and economic benefits?)*

Commercial contributions:

1. Patents, licenses, invention disclosures (Owen-Smith et al., 2001; Smilor et al., 2007; Grimaldi et al., 2011; NASEM, 2017a; Perkmann et al., 2011
2. Start-up companies (Smilor et al., 2007; Grimaldi et al., 2011)
3. Other products (Grimaldi et al., 2011)
4. Applications for GOALI, SBIR/STTR, Industry University Cooperative Research Centers (IUCRS), Innovation Corps, Partnerships for Innovation, or other NSF centers such as Science and Technology Centers (STC), Materials Research Science and Engineering Centers (MRSEC), or Engineering Research Centers (ERC)

Indicators	Data Source	Analytic Approach	Comparison Group
1-4	Open-ended data in Phase II internal and external program documents	Descriptive statistics of various products, with examples	None

2.2. In what ways have the CCIs developed partnerships to engage in technology transfer, to commercialize technology, or for other societal benefit?

Relationships with partners:

1. Number and types of partners (Smilor et al., 2007; NASEM, 2017a)
2. Nature of collaboration with industry (Perkmann et al., 2011)
3. Interest in commercialization (Trauth et al., 2015)
4. Alignment of research agenda to industry needs (Grimaldi et al., 2011; Nagle, 2007)
5. Funding from industry (McGowan, 2017)
6. Benefits to industry (Abt developed)
7. Industry experiences for students and staff (NASEM, 2017a; Lane, 2014)
8. Students moving to industry (NASEM, 2017a; Lane, 2014)

Indicators	Data Source	Analytic Approach	Comparison Group
1-2	Close-ended data in annual reports	Descriptive statistics of partners and turnover over time	None
3-6	Survey of CCI Phase I and II PIs and Co-Investigators, item 10 and item 14; interviews with industry partners	Descriptive statistics for survey items; summary of themes emerging from interviews	None
7-8	Survey of CCI students and postdocs, items 7-8 and 11-14	Descriptive statistics for survey items	None

Research Question 3: What are the contributions of the CCI Program in the areas of workforce development (education and professional development), broadening participation, and informal science communication?

3.1 What are the most important impacts of the CCIs in these three areas and how was this made possible (or enhanced) by the center mechanism of operation?

Workforce development activities:

1. Mentoring provided (Packard, 2012; Symonds et al., 2011)
2. Research and other experiential opportunities (Hunter et al., 2007; Piper et al., 2015; Seymour et al., 2004; Olson et al., 2012; Chubin 2010)
3. Informal student interactions (Piper et al., 2015)
4. Courses/seminars (Piper et al., 2015; Rodriguez et al., 2013)
5. Ability to attend conferences/symposia (Gardner et al., 2007; Piper et al., 2015; Seymour et al., 2004)
6. Ability to advance research and publish (Pinheiro et al., 2014; Chubin 2010)
7. Ability to take initiative or work on your own ideas (NSF suggested)
8. Opportunities to take on leadership responsibilities (NSF suggested)
9. Opportunities to collaborate with other researchers (Pinheiro et al., 2014)
10. Opportunities to participate in course development and teaching (Feldon et al., 2011)
11. Opportunities to mentor (Olson et al., 2012)
12. Opportunities to learn about commercialization (Chubin 2010)
13. Opportunities to network at conferences (NSF suggested)
14. Job opportunities and setting career direction (Abt developed)
15. Student and postdoc satisfaction with opportunities (Abt developed)
16. External perspective on broadening participation (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1-14	Survey of graduate students and postdocs, items 11-15; survey of PIs/Co-Investigators item 12; open-ended data in Phase I and II internal and external program documents; interviews with center PIs	Descriptive statistics for satisfaction ratings; Abstraction and coding of all relevant information; selected examples to include in Center profiles; summary of themes emerging from interviews	PIs on center grants (interview data)
15	Open-ended data in Phase II external program documents; interviews with individuals involved in oversight of CCIs	Abstraction of all relevant information; summary of external comments	None

Activities to broaden participation of under-represented minorities:

1. Recruitment/retention of URGs (Bensimon, 2004; Clewell et al., 2009; Garcia et al., 2001; Smith et al., 2006; Spencer, 2013)
2. Mentorship of URGs (Bensimon, 2004; Garcia et al., 2001; Smith et al., 2006)
3. Partnerships with HBCUs/MSIs and organizations that support URGs in science Clewell et al., 2009; Spencer, 2013)
4. Prepared/updated diversity plan (Clewell et al., 2009; Garcia et al., 2001; Smith et al., 2006)
5. Service on diversity committees (Smith et al., 2006)
6. External perspective on broadening participation (Abt developed)
7. Student experiences by subgroup (Clewell et al., 2009; Garcia et al., 2001; Smith et al., 2006)

Indicators	Data Source	Analytic Approach	Comparison Group
1-5	Open-ended data in Phase I and II internal and external program documents	Abstraction and coding of all relevant information; selected examples to include in Center profiles	None
6	Open-ended data in Phase II external program documents	Abstraction of all relevant information; summary of external comments	None
7	Survey of graduate students and postdocs, items	Descriptive statistics of satisfaction with various elements of CCI, disaggregated by gender and racial/ethnic minority (if sufficient data)	None

Activities aimed at informal science communication:

1. Community and outreach events, such as science cafes, museum exhibits, public lectures, etc. (Brownell et al., 2013; NASEM, 2017b; Nisbet & Markowitz, 2016)
2. Print, electronic/social media distributions (NRC, 2009; NASEM, 2016 and 2017b; Pavlov et al., 2018)
3. After-school programs (NRC, 2009)
4. Engagement with other organizations that host K-12 students (Abt developed)
5. Programs for science teachers (Abt developed)
8. Use of NSF media platforms/channels (Abt developed)
9. External perspective on informal science communication (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1-8	Open-ended data in Phase I and II internal and external program documents	Abstraction and coding of all relevant information; selected examples to include in Center profiles	None
9	Open-ended data in Phase II external program documents	Abstraction of all relevant information; summary of external comments	None

Role of CCI in broader impacts outcomes:

1. Indicators described above in the context of CCI funding (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
Workforce development	PI/Co-Investigator surveys item 12 and item 13; student/postdoc survey items 9-10 and 12-15	Descriptive statistics for survey items	None
Increased diversity	PI/Co-Investigator surveys item 12 and item 13	Descriptive statistics for survey items	None
Communicating with the public	PI/Co-Investigator surveys item 12; student/postdoc survey items 12, 14-15	Descriptive statistics for survey items	None

3.2 To what extent and in what ways are the CCIs providing leadership in these three broader impact areas?

External perspective on the leadership role of CCIs:

1. See indicators above

3.3 To what extent and in what ways have the CCIs contributed to sustained, institutionalized change in these three broader impact areas?

New infrastructure or collaborations developed/enhanced related to broader impact areas and expectation to sustain after CCI:

1. Evidence of sustainability of programs and partnerships created by CCIs (Abt developed)
2. Participant perspective on how CCIs have contributed to sustained institutional change (Abt developed)
3. External perspective on how CCIs have contributed to sustained institutional change (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1-2	Survey of CCI Phase I and II PIs and Co-Investigators, item 12; interviews with PIs	Descriptive statistics for survey items; summary of themes emerging from interviews	PIs on center grants (interview data)
3	Open-ended data in Phase II external program documents	Abstraction of all relevant information; summary of external comments	None

Research Question 4: How effective are the center structures and operations in achieving the program's goals?

4.1 What are some of the most effective center management strategies, and how are they adapted to their particular situations, in promoting?

Transformative outcomes?
Enhanced team integration and augmented productivity (synergy)?
Higher quality training opportunities for students and post-docs?
Increased diversity?
Improved public understanding and appreciation of chemistry?

Description of and satisfaction with center models:

1. Description of leadership, communication, data sharing strategies; center organization and partners; conflict resolution, credit sharing, and other policies (Hall et al., 2008; Vogel, 2012, Wuchty et al., 2007; Abt developed)
2. PI perception of the effectiveness of center structures and their role in achieving goals (Glied et al., 2007, Sonnenwald, 2004, Langfeldt et al., 2010, Ponomariov, 2010, Doussineau, 2014; Abt)
3. Challenges encountered and how these were resolved (Wuchty et al., 2007; Langfeldt et al., 2010; Vogel, 2012; Chubin, 2010; Hall, 2008; Wong-Parodi et al., 2014)

Indicators	Data Source	Analytic Approach	Comparison Group
1	Open-ended data in Phase II internal and external program documents	Abstraction and coding of all relevant information; selected examples to include in Center profiles	None
2	Survey of CCI Phase I and II PIs and Co-Investigators, items 15-23; interviews with PIs	Descriptive statistics for satisfaction ratings; summary of themes emerging from interviews	PIs on center grants (interview data)
3	Survey of CCI Phase I and II PIs and Co-Investigators, item 17; interviews with PIs	Descriptive statistics of challenges; summary of themes emerging from interviews	PIs on center grants (interview data)

4.2 (Modified) To what extent and in what ways have the CCIs influenced collaborations among center participants?) *(Original Question: To what extent and in what ways have the CCIs influenced and impacted collaborations among center participants*?)

Role of CCI in collaboration:

1. Level of pre-existing and current collaboration across partner organizations and role of CCI (Boardman & Corley, 2008))
2. Expectation to maintain most or all collaborations after the grant (Abt developed)
3. Persistence of collaboration among the Phase I CCIs which did not receive Phase II funding (Abt developed)
4. Types of partners and changes to partners over time (Abt developed)
5. External perspective on the role of collaborations (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1-4	Survey of CCI Phase I and II PIs and co-investigators, items 6-8; interviews with PIs	Descriptive statistics of survey items; summary of themes emerging from interviews	PIs on center grants (interview data)
5	Open-ended data in Phase II external program documents	Abstraction of all relevant information; summary of external comments	None

4.3 To what extent and in what ways have the CCIs made use of tools and communication to facilitate collaboration?

Tools used by CCIs:

1. Types of tools, such as online discussion forums, shared depositories for code and data, virtual conferencing, collaborative editing of documents, center website (Abt developed)
2. Satisfaction with collaborative tools (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1	Open-ended data in Phase II internal and external program documents	Abstraction and coding of all relevant information; selected examples to include in Center profiles	None
2	Survey of CCI Phase I and II PIs and Co-Investigators, items 11 and 15; interviews with PIs	Descriptive statistics of satisfaction ratings; summary of themes emerging from interviews	PIs on center grants (interview data)

Research Question 5: How effective is the 2-phase funding model for the CCI Program?

5.1 What are the strengths and weaknesses of the 2-phase award process?

5.2 What is the value of the Phase I award experience for the awardees?

Satisfaction with the 2-phase process:

1. CCI grantee perspective on advantages and disadvantages of the concept (Abt developed)
2. CCI grantee perspective on the specifics of the model, such as length of each phase and funding level (Abt developed)
3. Value of Phase I to grantees who did and did not receive Phase II funding (Abt developed)
4. Single-phase grantee perspective on the two-phase model (Abt developed)
5. External perspective on the 2-phase model (Abt developed)

Indicators	Data Source	Analytic Approach	Comparison Group
1-4	Survey of CCI Phase I and II PIs and Co-Investigators, items 9-10, 15-23; interviews with PIs	Descriptive statistics of satisfaction with 2-phase process; summary of themes emerging from interviews	PIs on center grants (interview data)
5	Open-ended data in Phase II external program documents; interviews with individuals involved in oversight of CCIs	Abstraction of all relevant information; summary of external comments; summary of themes emerging from interviews	None

B.2 Notes on Data Sources and Analytic Approach

Publications

- *Data collection and analysis*: We will abstract all publications listed in Phase I and Phase II annual reports using a semi-automated approach. All authors on these publications will be matched to a CCI list of participants to identify grantees and non-grantees. Author names will then be used to query the Scope database to collect additional publications. Bibliometric indicators (e.g., counts of publications, citations, author affiliations) will be obtained for the period before, during, and after CCI participation. Additionally, a collaboration network for CCI participants will be developed based on co-authorships and the best performers identified.

- *Comparison Group*: A sample of PIs on individual chemistry grants funded by the NSF Chemistry Division will be used. Comparisons will allow us to make statistical inferences about the differences between CCI grantees and other chemists funded by NSF, but we will not be able to link these differences to CCI participation due to the possibility of confounding variables.

Patents

- *Data collection and analysis*: We will abstract all patents listed in Phase I and Phase II annual reports as described for publications. In addition, CCI publications cited in awarded US patents will also be identified through matching.

- Comparison group: None

Other Systematic Annual Report Data

- *Data collection and analysis*: Data scraping will be used to abstract basic information on participants, partners, and products prepared other than publications and patents (e.g., books or book chapters, theses/dissertations, inventions, licenses, websites, other technologies). Simple descriptive statistics will be performed on these data.

- *Comparison Group*: None

Open-ended Data

- *Types of sources:* Program documents refer to *internal documents* (annual reports and proposals) and *external documents* (oversight/funding memos, site visit reports, internal interim reviews, and committee of visitor reports).
- *Data collection and analysis*: We will review all Phase II internal and external program documents and abstract information into an Access database. We will use pre-determined codes to document the presence of a given indicator, and open fields to provide brief descriptions of selected instances. For external documents, we will create special indicators to reflect whether the views conveyed about the center by reviewers are positive, negative, or mixed. Selected examples of center programs, processes, and activities which seem particularly innovative and/or impactful and/or highlighted by external reviewers will be flagged, and included in a profile developed for each of the Phase II Centers.
- *Comparison group*: None

Surveys of CCI PIs/Co-Investigators and Students/Postdocs

- *Data collection and analysis:* We will conduct online surveys of all PIs and Co-Investigators (i.e., Primary PI, PD/PI, Co PD/PI, Co-Investigator, Senior Personnel indicated in annual reports) of Phase I and Phase II awards and of all graduate students/postdocs who were included in annual reports between the 2012-13 and 2016-17 reporting years. Data collected in the survey will be analyzed using descriptive statistics, and stratified by phase and participant characteristics, as relevant.
- *Comparison group*: Selected items will be benchmarked to other surveys to the extent possible. However, due to differences in contexts between the programs, timing of data collection, and minor changes to survey items, it will not be possible to understand what led to these differences if they emerge.

Interviews with Phase II PIs/Co-Investigators, Comparison PIs, Industry Partners, and Individuals Involved in Oversight Activities of CCIs

- *Data collection and analysis:* We will interview a sample of Phase II CCI PIs/Co-Investigators to better understand the contributions of their centers, strengths and weaknesses of the center structure and a two-phased funding model, and other areas which cannot be easily captured in a survey. Additionally, we will interview industry partners, to further capture how they benefit from the centers, and PIs on other centers, to get their perspective on a two-phase vs one-phase strategy and understand their key accomplishments. Finally, we will interview participated in site visits or oversight activities of CCI centers, including both NSF staff and external experts, to get an external perspective on CCI implementation and outcomes. We will also code and summarize major themes that emerge from open-ended survey items and from interviews.
- *Comparison group*: Interviews will be conducted with investigators from other centers to compare processes and outcomes of CCI to other centers. Due to the small sample size and differences in the programs, these comparisons will be qualitative and primarily provide general context.

Appendix C: Patents Cited in CCI Reports

Patent Number	Year Granted	Funding Acknowledged	Title
US8192609B2	2012	NSF 0802907	Cobalt oxyfluoride catalysts for electrolytic dissociation of water
US8436337B2	2013	US Army: W911NF-07-2-0083, W909MY-06-C-0038	Amorphous multi-component metallic thin films for electronic devices
US9340678B2	2016	US Air Force FA8650-05-1-5041	Process to form aqueous precursor and aluminum oxide film
US9511585B2	2016	No	Thermal inkjet printhead stack with amorphous thin metal protective layer
US8362312B2	2013	NSF CHE-0107810	Supported iridium catalysts
US8585888B2	2013	NSF CHE-0650456	Copper-based water oxidation catalysts
US9260367B2	2016	NSF CHE-0650456, CHE-1205189, CHE-0836095	Methods of converting polyols
US9315604B2	2016	NSF CHE-1111133, DOE DE-FG02-86ER13564	Metathesis catalysts and methods thereof
US9770710B2	2017	NSF CHE-0650456, CHE-1205189	Hydrogenation and disproportionation catalysis
US9802971B2	2017	No	Alkane dehydrogenation process
US9902673B2	2018	NSF 1205189	Methods for producing butanol
US8975428B2	2015	NSF CHE 0750273	Dirhodium catalyst compositions and synthetic processes related thereto
US9315477B2	2016	NSF CHE-1205646	Materials having electron deficient moieties and methods of synthesizing thereof
US9556080B2	2017	NSF CHE-1205646, CHE-1212767	Silylation of aromatic heterocycles by disilanes using potassium alkoxide catalysts
US10161051B2	2018	NSF CHE-1240020	Electrochemical reduction of CO2 at copper nanofoams
US9234285B2	2016	NSF CHE1240020	Electrochemical processing of clathrate hydrates
US9371347B2	2016	NSF CHE-1240020	dppf-like compounds and method of manufacture and use
US9834490B1	2017	No	Solar-enriched biofuels via looped oxide catalysis
US8956525B2	2015	NSF 0802907	Buffered cobalt oxide catalysts
US8626449B2	2014	NSF ATM0321362	Biological cell sorting and characterization using aerosol mass spectrometry
US9505778B2	2016	NSF CHE-1136607	Monomers, polymers and articles containing the same from sugar derived compounds
US9624314B2	2017	NSF CHE-1413862	Porous cyclodextrin polymeric materials and methods of making and using same
US9718763B2	2017	NSF	Catalytic ester decarbonylation
US9815808B2	2017	NSF CHE-1413862	Recovery of monomer from polyurethane materials by depolymerization
US9988393B2	2018	NSF CHE-1413862	Isosorbide-based polymethacrylates
US8904561B2	2014	NIH HG-04431, HG-04549	Mechanical detection of Raman resonance
US9658162B2	2017	NSF CHE-0802913	Method and apparatus for direct measurement of the amplitude and/or phase of a molecular vibration
US9375790B2	2016	No	Continuous flow reactor and method for nanoparticle synthesis

Appendix D: Comparison Award Program Element Codes

Program Element Code	Program Name
2004-2009	
1942	UNIMOLECULAR PROCESSES
1944	BIMOLECULAR PROCESSES
1948	SYNTHESIS
1950	METHODOLOGY
1954	QUANTUM CALCULATIONS
1956	STATISTICAL AND SIMULATIONS
1960	STRUCTURE AND REACTIVITY
1962	SPECTROSCOPY
1966	SYNTHETIC INORGANIC
1968	PHYSICAL INORGANIC
1972	ELECTROCHEMISTRY & SURFACE CHE
1974	ANALYTICAL SEPARATIONS & MEAS.
2009-2016	
6878	CHEMICAL SYNTHESIS (SYN)
6880	CHEMICAL MEASUREMENT & IMAGING (CMI)
6881	THEORY, MODELS, COMPUT. METHOD (CTMC)
6882	ENVIRONMENTAL CHEMICAL SCIENCE (ECS)
6883	CHEMISTRY OF LIFE PROCESSES (CLP)
6884	CHEMICAL CATALYSIS (CAT)
6885	MACROMOLEC/SUPRAMOLEC/NANO (MSN)
9101	CHEM STRUCT,DYNMCS&MECHANSMS A (CSDM A)
9102	CHEM STRUCT,DYNMCS&MECHANSMS B (CSDM B)

2009-2013: CSDM A/B = CSDM

Appendix E: Data Collection Instruments

E.1 Survey of Principal Investigators and Co-Investigators

OMB# 3145-NEW

Pilot only:
Thank you for agreeing to help pilot test this survey. Your feedback will help us improve the survey before we send it to other CCI participants.

Please review the instructions on this page and the next before beginning. On each page of the survey we have included a text box for you to add comments about any questions that are not clear or relevant to you. You only need to fill in these text boxes for any survey items for which you have specific comments. At the end of the survey, we have included a brief set of questions on your overall impressions of the survey's content, clarity, and length.

All respondents:
This survey solicits responses from all lead Principal Investigators and Co-Investigators participating in the National Science Foundation's (NSF) Centers for Chemical Innovation (CCI) Program. The goal of the survey is to inform the evaluation of the program. We are asking for information to supplement your annual reports. All data will be aggregated to not reveal individual respondents. The survey should take no more than 20 minutes to complete.

INSTRUCTIONS

- Please use the survey's navigation buttons ("Back" and "Next") to move through the questionnaire.
- You may exit the survey at any time by pressing the "save and continue later" button. When you re-open the survey, you will be able to continue where you left off.
- Once you reach the last question in the survey, you will see a "submit" button. After clicking this button, your survey will be complete and you may close your browser. Once submitted, you will not be able to return to the survey without contacting our team.
- If you have any questions regarding the survey, you can contact us at CCISurvey@abtassoc.com.

[Verification]

1. **Is your name: [First Name, Middle Name/Initial, Last Name]?**
   - ☐ Yes, this is correct
   - ☐ No, my name has changed or is misspelled. My name is: _________
   - ☐ No, I'm not the person named above → Exit the survey

2. **All of the questions in the survey refer to your participation in the following NSF Center for Chemical Innovation (CCI): [CCI name].**
   Please note that when first established, the program was called the Chemical Bonding Centers.
   - ☐ I have participated in this CCI → 3
   - ☐ I have not participated in this CCI, but I have participated in a different CCI → A
   - ☐ I have not participated or I am not sure whether I participated in the CCI Program → Exit

   A. **Please select from the list of options.**
   If you participated in more than one CCI, please select the CCI with which you have been most extensively involved and limit your answers to this CCI only.
   [pull-down menu of CCIs]

3. **For how many years have you been or were you associated with the CCI Program?**
   - ☐ <1 year
   - ☐ 1 year
   - ☐ 2 to 4 years
   - ☐ 5 to 6 years
   - ☐ 7 or more years

[Project characteristics]

4. **On a scale of 1-5, where 1 indicates "not at all" and 5 indicates "very," to what extent does the research conducted by your CCI have the following characteristics? Enter one response per row.**

	1-5
Addresses important societal problem	
Focuses on major scientific challenge(s) in fundamental chemistry	
Has the potential to radically change our understanding of an important scientific or engineering concepts	
Interdisciplinary	
High-risk	
Requires a coordinated effort from diverse experts	
Requires large investment of funds	

[Pre-existing collaboration and role of CCI in collaboration]

5. Had you collaborated with any or all of the CCI partners before the center was established? Select one.

- ☐ None of the partners → 9
- ☐ Some of the partners → 7
- ☐ Half or more of the partners → 7

6. To what extent has participation in CCI influenced these pre-existing collaborations? Select one.

- ☐ Not at all
- ☐ To some extent
- ☐ To a considerable extent

7. Have you continued or do you expect to continue collaborating with CCI partners after the end of the grant? Select all that apply.

- ☐ No
- ☐ I maintained or expect to maintain some CCI collaborations after the grant ends
- ☐ I maintained or expect to maintain most or all CCI collaborations after the grant ends
- ☐ Uncertain

[Benefits of CCI participation: research, personal visibility, and infrastructure for the community]

8. Please indicate whether participation in the CCI has benefited your research program. Select one response per row.

	No Benefit Due to CCI	Some Benefit Due to CCI	Large Benefit Due to CCI	Not Applicable
Use of new theoretical models				
Use of new/additional instrumentation or technology				
Use of new/additional data sources				
Use of new/additional theoretical or experimental models				
Ability to generate new and/or better ideas				
Ability to more quickly/effectively respond to scientific developments				
Ability to take your research in a new direction				
Access to resources at partner institutions				
Access to resources at your institution				
Ability to attract better qualified or more diverse students and postdocs to your research group				
Ability to obtain additional funding to support your research				

9. Have any of the following changes occurred in your publication patterns, research interests, and/or professional visibility since you began participating in CCI? Select one response per row.

	Decreased Due to CCI Participation	Decreased, but Not Due to CCI Participation	Has Not Changed/ Too Early to Tell	Increased, but Not Due to CCI Participation	Increased Due to CCI Participation
Number of papers published per year					
Journal quality					
Publishing in a broader range of journals					
Publishing with industry					
Funding from industry					
Interest in commercialization					
Participation in new professional conferences, associations or societies					
Number of speaking invitations					
Requests to serve on dissertation committees outside your home institution					
Requests to serve on advisory panels					
Requests to serve on editorial boards of journals					
Requests to serve as a peer reviewer					
Requests to provide policy advice or testimony					
Receipt of awards, fellowships, or chaired positions					
Diversity of research problems on which you work					

10. Which of the following resources/infrastructure created or improved by CCI, if any, are being used by researchers <u>not affiliated with the center</u>? Select all that apply.

- ☐ Methods
- ☐ Reagents
- ☐ Data
- ☐ Communication infrastructure
- ☐ Data management system
- ☐ Educational or outreach materials
- ☐ Facilities
- ☐ Equipment
- ☐ Lessons learned for how to run a large center
- ☐ New partnerships
- ☐ Other resources. Please specify: __________
- ☐ I am not aware of any resources created or improved by CCI that are being used by researchers not affiliated with the center

[Benefits of CCI participation: broader impacts]

11. Please indicate whether your CCI developed or improved the following educational or outreach opportunities

- ☐ Courses/seminars in chemistry
- ☐ Training programs in chemistry
- ☐ Research and teaching experiences for students and postdocs
- ☐ Programs for educating the public about chemistry
- ☐ Mechanisms for recruitment and/or retention of individuals from underrepresented groups [hyperlink defining URGs]
- ☐ Mechanisms for mentorship of individuals from underrepresented groups
- ☐ Engagement with organizations with expertise supporting underrepresented groups in the scientific community
- ☐ Engagement with organizations focused on STEM-related outreach and advocacy
- ☐ I do not know whether my CCI developed or improved these types of opportunities → skip to Q13

[URGs include women, members of racial and ethnic minorities, persons with disabilities, and persons with low socio-economic status]

12. **Current grants: Please indicate whether you expect to be able to sustain the following programs and activities after the grant ends.**
Completed grants: Please indicate whether the following programs and activities are still in place.
    - ☐ Courses/seminars in chemistry
    - ☐ Training programs in chemistry
    - ☐ Research and teaching experiences for students and postdocs
    - ☐ Programs for educating the public about chemistry
    - ☐ Mechanisms for recruitment and/or retention of individuals from underrepresented groups [hyperlink defining URGs]
    - ☐ Mechanisms for mentorship of individuals from underrepresented groups
    - ☐ Engagement with organizations with expertise supporting underrepresented groups in the scientific community
    - ☐ Engagement with organizations focused on STEM-related outreach and advocacy

[URGs include women, members of racial and ethnic minorities, persons with disabilities, and persons with low socio-economic status]

13. **Please indicate whether the following improvements have occurred as a result of CCI funding. Select one response per row.**

	No Improvement Due to CCI	Some Improvement Due to CCI	Large Improvement Due to CCI	N/A
Increased participation of underrepresented groups in your lab				
Increased participation of underrepresented groups at your institution				
Improved ability of students and postdocs to obtain a position after leaving CCI				
Improved quality of education in chemistry				
Increased interest in/understanding of chemistry among the public you were able to reach				

14. Please indicate whether the CCI delivered any of the following benefits to industry. Select one response per row.

☐ I am not aware of any partnerships between my CCI and industry → skip table below

	No Benefit Due to CCI	Some Benefit Due to CCI	Large Benefit Due to CCI	Uncertain
New or improved ideas for commercial product or process				
New or improved product or process				
Reduction in environmental impact				
Ability to meet regulatory requirements				
Access to personnel				
Increase in sales				
Cost savings				
Other benefits. Please specify: ______________				

[Center organization and function]

15. On a scale of 1-5, where 1=least and 5=most, how satisfied are you with the following elements of CCI?

	N/A	1=Least	2	3	4	5=Most
Requirement to develop a strategic plan						
Distribution of resources among partners						
Sharing of credit among partners						
Intellectual contribution of partners						
Productivity of meetings among partners						
Frequency of meeting among partners						
Communication tools						
Data sharing tools						
Professional development opportunities for students/postdocs						
Broadening participation activities and programs						
Public outreach activities and programs						
Leadership of the center						
Overall direction of the center						
Funding level for Phase I *(Display for Phase I only)*						
Funding level for Phase II *(Display for Phase II only)*						
Duration of Phase I *(Display for Phase I only)*						
Duration of Phase II *(Display for Phase II only)*						

16. To what extent have these elements contributed to the success of your center?

	None	Some	Considerable
Requirement to develop a strategic plan			
Distribution of resources among partners			
Sharing of credit among partners			
Intellectual contribution of partners			
Productivity of meetings among partners			
Frequency of meeting among partners			
Communication tools			
Data sharing tools			
Professional development opportunities for students/postdocs			
Broadening participation activities and programs			
Public outreach activities and programs			
Leadership of the center			
Overall direction of the center			
Funding level for Phase I *(Display for Phase I only)*			
Funding level for Phase II *(Display for Phase II only)*			
Duration of Phase I *(Display for Phase I only)*			
Duration of Phase II *(Display for Phase II only)*			

17. Overall, how would you rate your experience in the CCI? Select one.

- ☐ Very satisfied
- ☐ Satisfied
- ☐ Neutral
- ☐ Dissatisfied
- ☐ Very dissatisfied

18. Has your CCI experienced the following challenges? Select all that apply.

- ☐ Technical or experimental
- ☐ Meeting administrative requirements
- ☐ Sharing of credit for discovery
- ☐ Communication between partners
- ☐ Coordination of activities between partners
- ☐ Contributions by partners to the center
- ☐ Delays in progress of research
- ☐ Staffing of the center
- ☐ Access to needed resources
- ☐ Seeding new projects
- ☐ Terminating unsuccessful projects
- ☐ Other challenge. Please specify: _____

19. **To what extent have these challenges been resolved?**

Challenge	Not at All	To Some Extent	Fully
Technical or experimental			
Meeting administrative requirements			
Sharing of credit for discovery			
Communication between partners			
Coordination of activities between partners			
Contributions by partners to the center			
Delays in progress of research			
Staffing of the center			
Access to needed resources			
Seeding new projects			
Terminating unsuccessful projects			
Other challenge. Please specify:			

20. **Phase II only: To what extent has participation in Phase I contributed to the success of your Phase II center? Select one.**
    - ☐ I did not participate in Phase I → skip to "In your view…" (Q23)
    - ☐ Not at all
    - ☐ To some extent
    - ☐ To a considerable extent
21. **Have any of the following occurred <u>as a result of your participation in Phase I</u>? Select all that apply.**
    - ☐ Advanced your research program
    - ☐ New direction for your research program
    - ☐ Formed new or cemented old collaborations
    - ☐ Obtained additional funding to support your research
    - ☐ Gained experience participating in or running a center
    - ☐ Developed center policies and procedures
    - ☐ Developed educational or public outreach programs
    - ☐ Provided training or career development opportunities for students or postdocs
    - ☐ Other benefits. Please describe:_____
    - ☐ No benefits of participation in Phase I
22. **Phase I only: Have you been able to continue working on the CCI-funded projects? Select one.**
    - ☐ Yes
    - ☐ No

23. In your view, which of the following are the <u>advantages</u> of the 2-phase model? Select all that apply.

- ☐ It enables selection of better Phase II centers by NSF
- ☐ It allows participants to determine whether they like the experience
- ☐ It allows selection of the right partners
- ☐ It allows the centers to refine their research goals and approach
- ☐ It allows the centers to pilot activities and programs
- ☐ It allows the centers to develop and test policies and procedures
- ☐ No advantages
- ☐ Other advantages. Please specify:____________

24. In your view, what are the <u>disadvantages</u> of the 2-phase model? Select all that apply.

- ☐ Some strong applicants may be discouraged from applying
- ☐ Insufficient resources for Phase I grantees not selected for Phase II to continue their research
- ☐ Time burden to submit a Phase II application
- ☐ Delay in tacking time-sensitive topics
- ☐ Other disadvantages. Please specify:_____________
- ☐ No disadvantages

25. On balance, is a 2-phase center model preferable to a single phase? Select one.

- ☐ Yes, 2-phase model is preferable
- ☐ No, 1-phase model is preferable
- ☐ Uncertain

E.2 CCI Graduate Student and Postdoctoral Researcher Survey

This survey solicits responses from graduate students and postdocs who have participated or are currently participating in the National Science Foundation's (NSF) Centers for Chemical Innovation (CCI) Program. The survey is part of the external program evaluation, which aims to understand the role of the CCIs in graduate and postdoctoral training and career development. All survey responses will be aggregated to not reveal individual identities. The survey should take no more than 15 minutes to complete.

CONSENT

Participation in the survey is voluntary, and nonparticipation, discontinuing the survey, or skipping questions will have no impact on you. All information that would permit identification of an individual respondent will be held in confidence, will be used by only persons engaged in and for the purpose of the survey, and will not be disclosed or released to others for any purpose except as required by law. Information from the survey will only be reported in the aggregate at the program level, combined with other responses. While there are no direct benefits of your participation in this survey, your frank and open responses will help the National Science Foundation to strengthen the design and operation of the program. The evaluation will also communicate the impacts of the CCI Program to the chemistry community. Hence, we encourage you to respond candidly about your experiences.

INSTRUCTIONS

- Please use the survey's navigation buttons ("Back" and "Next") to move through the questionnaire.
- You may exit the survey at any time by pressing the "save and continue later" button in the gray bar at the top of the window. When you re-open the survey, you will be able to continue where you left off.
- Once you reach the last question in the survey, you will see a "submit" button. After clicking this button, your survey will be complete and you may close your browser. Once submitted, you will not be able to return to the survey without contacting our team.
- A small number of questions in the survey are required, either to confirm that the survey was sent to the correct person or to allow for logical follow-up questions. These questions are indicated with an asterisk (*). You will not be able to proceed to the next question without answering these required questions.
- If you have any questions regarding the survey or you experience technical challenges, you can contact us at NSF_CCI@abtassoc.com.

The OMB control number for this project is 3145-0250. Public reporting burden for this collection of information is estimated to average 15 minutes per respondent, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspects of this collection of information, including suggestions for reducing this burden, to Suzanne H. Plimpton, Reports Clearance Officer, National Science Foundation, 2415 Eisenhower Ave, Alexandria, VA 22314 or send e-mail to splimpto@nsf.gov.

[Verification]

Past and current:

1. **Is your name: [First Name, Last Name]? ***

    ☐ Yes, this is correct

    ☐ No, my name has changed or is misspelled. My name is: __________

    ☐ No, I am not the person named above → Exit the survey

Past and current:

2. **All of the questions in the survey refer to your participation in the following NSF Center for Chemical Innovation (CCI): [CCI name] ***
    Please note that when first established, the program was called the Chemical Bonding Centers.

    ☐ I have participated/am still participating in this CCI → 3

    ☐ I have not participated/am not participating in this CCI, but I have participated/am still participating in a different CCI → A

    ☐ I have not participated or I am not sure whether I participated in the CCI Program → Exit the survey

    A. **Please select from the list of options ***
    If you participated in more than one CCI, please select the CCI with which you have been most extensively involved and limit your answers to this CCI only.
    [pull-down menu of CCIs]

Past and current:

3. **Are you still part of this CCI? Select one. ***

    ☐ Yes → current

    ☐ No → past

Past and current:

4. **For how long [current: have you been / past: were you] associated with the CCI Program?**

    ☐ 3 or fewer months

    ☐ 4 to 6 months

    ☐ 7 to 11 months

    ☐ 1 year

    ☐ 2 to 3 years

    ☐ 4 or more years

    ☐ Uncertain/do not recall

Past only:

5. Why are you no longer participating in CCI? Select all that apply.

- ☐ Graduated/completed postdoctoral training → 6
- ☐ Left for another reason → A

A. Please indicate all reasons that apply.

- ☐ Insufficient funding
- ☐ Advisor left the CCI
- ☐ Completed CCI-related project and moved on to a project not related to CCI
- ☐ Was assigned to a different project
- ☐ Was not interested in research being conducted
- ☐ Did not get along with advisor/inadequate mentoring
- ☐ Did not get along with people in the center
- ☐ Did not get resources I needed
- ☐ Decided to pursue another career path
- ☐ Did not like being part of a center
- ☐ Left graduate/postdoctoral program before completion
- ☐ Personal/family reason or change in life circumstances
- ☐ Other, please explain: ____________

[Career status and plans]

Past and current:

6. [current: Are / past: During your final year at CCI, were] you:

- ☐ A terminal masters student → A (if current), 7 (if past)
- ☐ A doctoral student → 7
- ☐ A postdoctoral scholar → 7
- ☐ Other, please explain: _______________ → 7

Current only:

A. After you graduate, are you planning to pursue a PhD?

- ☐ Yes → B
- ☐ No → C
- ☐ Unsure → 7

B. Has your CCI experience positively influenced your interest in pursuing a PhD?

- ☐ Yes, it increased my interest in pursuing a PhD → 7
- ☐ No, I was already planning to pursue a PhD → 7

C. Has your CCI experience negatively influenced your interest in pursuing a PhD?

☐ Yes, it decreased my interest in pursuing a PhD → 7

☐ No, I was not planning to pursue a PhD → 7

Past and current:

7. How many people [past: served / current: serve] as mentors to you (either formally or informally), providing guidance, feedback, and support for your development and research? Select one.

☐ I [past: had / current: have] a single mentor who [past: participated /current: participates] in CCI

☐ I [past: had / current: have] a single mentor who [past did / current: does] not participate in CCI

☐ I [past: had / current: have] multiple mentors who all [past: participated / current: participate] in CCI

☐ I [past: had / current: have] multiple mentors, but not all of them [past: participated / current: participate] in CCI

☐ I [past: did / current: do] not have any mentors

Past only:

8. Did your CCI experiences influence any of these choices? Select all that apply.

☐ Type of institution to join – e.g., university, industry, government

☐ Type of career to pursue – e.g., research, teaching, entrepreneurship

☐ Whether to pursue a doctoral or professional degree –

☐ Whether to pursue postdoctoral training

☐ Choice of specific employer

☐ Choice of discipline/field of study

☐ Choice of research problem

☐ Choice of advisor/mentor

Past only:

9. Are you currently enrolled in a degree program? Select one.

☐ Yes → A

☐ No → 10

A. Is your degree program in chemistry or a related field?

☐ Yes → 12

☐ No → 12

Past only:

10. Which of the following best describes your current principal employer? Select one.

- ☐ Not employed
- ☐ College or university
- ☐ Industry (chemical or pharmaceutical company or similar)
- ☐ Government (including government research labs)
- ☐ Non-government lab
- ☐ Research institution/think tank
- ☐ Other nonprofit organization or private foundation
- ☐ K-12 school or district
- ☐ Entrepreneur/self-employed
- ☐ Other, please specify: ______

Current only:

11. Which of the following positions are you most interested in pursuing after you complete your degree and/or postdoctoral training? Have your career goals changed since you began participating in the CCI? Select one answer per row.

	Never Been My Goal	Considered before Involvement in CCI	Became a Goal Since Involvement in CCI
Faculty member in a research college or university			
Faculty member in a 2-year or 4-year teaching college			
Program officer/academic administrator			
Non-tenure-track researcher in a university or a research institute			
Researcher in a government laboratory			
Research and development position in industry			
Business position in industry or an entrepreneur			
Science policy, law, consulting, or science writing			
Other, please specify:			

[Experience with CCI]

Past and current:

12. [past: Did you spend time / current: Have you spent time] working in a laboratory/research group of another CCI partner organization (e.g., another university or company involved with your center) as an intern, graduate student, visiting scholar, or similar role? Select one.

- ☐ Yes → A
- ☐ No → 14

A. **Which of the following best describes the partner organization(s) in which you worked and/or currently work? Select all that apply if you worked with more than one type of organization.**

- ☐ Academic institution
- ☐ Government laboratory
- ☐ Industry
- ☐ Foundation/non-profit
- ☐ Other, please specify: ______________

B. **How much time did you work at CCI partner organization(s) in total?**
Enter number _____ [Pull down menu for weeks/months/years]

C. **How valuable was this experience to your career development? Select one.**

- ☐ Not at all valuable
- ☐ Somewhat valuable
- ☐ Very valuable
- ☐ Too early to tell/uncertain

Past and current:

13. Which of the following professional development opportunities offered through your CCI [past: did you experience / current: have you experienced]? Select all that apply.

- ☐ Mentorship
- ☐ Research opportunities
- ☐ Internships/visits to other research labs
- ☐ Attending conferences
- ☐ Giving presentations
- ☐ Publishing papers
- ☐ Applying for grants/fellowships/awards
- ☐ Collaborating with researchers at your institution
- ☐ Collaborating with researchers outside of your institution
- ☐ Entrepreneurship
- ☐ Teaching and/or course development
- ☐ Supervising students
- ☐ Outreach to the general public

14. How satisfied [past: were / current: are] you with these opportunities?

	Very Dissatisfied	Dissatisfied	Neutral	Satisfied	Very Satisfied
Mentorship					
Research opportunities					
Internships/visits to other research labs					
Attending conferences					
Giving presentations					
Publishing papers					
Applying for grants/fellowships/awards					
Collaborating with researchers at your institution					
Collaborating with researchers outside of your institution					
Entrepreneurship					
Teaching and/or course development					
Supervising students					
Outreach to the general public					

Past and current:

15. Overall, how would you rate your experience in the CCI? Select one.

- ☐ Very dissatisfied → A
- ☐ Dissatisfied → A
- ☐ Neutral → 16
- ☐ Satisfied → 16
- ☐ Very satisfied → 16

A. What is the primary reason for your dissatisfaction?

____

[Role of CCI]

Past and current:

16. Please indicate, for each item below, whether participation in CCI has proved to be an advantage, disadvantage, or made no difference:

	An Advantage	No Difference	A Disadvantage	NA/Too Early to Tell
Breadth of research experience				
Access to equipment, facilities, materials, reagents				
Ability to advance your research project				
Ability to develop/work on your own ideas				
Opportunities to take on leadership responsibilities				
Access to faculty				
Learning about scientific or engineering areas outside of your field				
Learning about commercialization and entrepreneurship				
Learning how to communicate about your research				
Quality of education				
Quality of training				
Quality of mentoring				
Access to community of peers				
Opportunities to network				
Determining your career direction and options				
Job opportunities available to you				

Past and current:

17. How well do you think participation in the CCI [past: has prepared / current: is preparing] you for the following activities? Choose one answer per row.

	Not Prepared	Somewhat Prepared	Well Prepared	N/A/Too Early to Tell
Formulating research problems				
Critically evaluating published literature				
Conducting high-quality research				
Solving problems which arise in implementing a research program				
Presenting and publishing your work				
Working in a multidisciplinary team				
Working outside of academia				
Writing fellowship/grant proposals				
Communicating with researchers in your field				
Communicating with researchers outside of your field				

	Not Prepared	Somewhat Prepared	Well Prepared	N/A/Too Early to Tell
Communicating research findings to the general public				
Serving as a mentor				
Teaching				

[Demographics]

Past and current:

18. What is your gender?

- ☐ Male
- ☐ Female
- ☐ Prefer not to report

Past and current:

19. Do you identify as an underrepresented ethnic/racial minority?

- ☐ Yes → A
- ☐ No → End of the survey
- ☐ Prefer not to report → End of the survey

A. If so, indicate:

- ☐ Black or African American
- ☐ Hispanic/Latino
- ☐ Native American
- ☐ Alaska Native
- ☐ Native Pacific Islander
- ☐ Prefer not to report
- ☐ Other. Please specify ___________

E.3 Interviews with CCI Lead PIs

Interview Consent and OMB Notification

Thank you so much for making time today to talk with me about NSF-funded Center-based research programs. We are interviewing a sample of Principal Investigators from across NSF's center-based research community. Your feedback will inform NSF on issues relevant to the design, implementation, and evaluation of center-based research programs.

Your answers will be aggregated with these of other respondents and the information you provide will not be attributed to you personally. Your participation is voluntary. Please feel free to skip any question you do not want to answer.

We would like to audio-record this interview to make sure we accurately capture everything you say. These recordings will not be shared outside of our team and will be destroyed in the end of the study. [If using a note taker] My colleague, [name], is on the telephone with me; [he/ she] will help me take notes during the interview. Is that okay?

[If audio taping the interview]: We would like to audio-record this interview as well to make sure we accurately capture everything you say. These recordings will not be shared outside of our team and will be destroyed in the end of the study. Is that okay with you?

Do you have questions for me before we proceed?

Additional information if needed. You do not need to read:

The OMB control number for this project is 3145-0215. Public reporting burden for this collection of information is estimated to average 60 minutes per respondent, including the time for consenting. Send comments regarding this burden estimate or any other aspects of this collection of information, including suggestions for reducing this burden, to Suzanne H. Plimpton, Reports Clearance Officer, National Science Foundation, 2415 Eisenhower Ave, Alexandria, VA 22314 or send e-mail to splimpto@nsf.gov.

Introduction

1. Why did you decide to participate in the CCI Program?

Accomplishments

2. What do you see as the most important scientific accomplishments of the Center (please describe in non-technical language if possible)? To what extent have these accomplishments been made possible by the Center?
3. What do you see as the most important non-scientific accomplishments of the Center? To what extent have these accomplishments been made possible by the Center?
4. Has your Center evolved in unexpected ways and/or deviated from the original goals? If yes, in what way and what were the consequences of these changes?
5. What programs, partnerships, and processes created by the Center do you think will remain after the funding ends?

Center Model

6. In your opinion, are there certain types of problems that are better suited to the Center funding mechanism? Which of these characteristics apply to your Center?
7. Did the Center structure enable your center to more rapidly respond to scientific developments in the field? If yes, can you give some examples?
8. What are the characteristics of a successful partner and partnership? Which partnerships do you see as the most and least successful?
9. What processes, policies, and other organizational components of your Center do you see as the most effective?
10. What have been the main challenges for your Center? What would you do differently if you could start again?
11. What do you see as the main advantages and limitations of the Center model? Of the 2-phase funding mechanism?
12. In hindsight, do you think a 1-phase or 2-phase mechanism would have been more effective for your center? Should NSF maintain this mechanism for future centers?
13. Has being part of the Center changed the direction, visibility, and productivity of your research group?

E.4 Interviews with CCI Managing Directors

Interview Consent and OMB Notification

Thank you so much for making time today to talk with me about NSF-funded Center-based research programs. We are interviewing a sample of Principal Investigators from across NSF's center-based research community. Your feedback will inform NSF on issues relevant to the design, implementation, and evaluation of center-based research programs.

Your answers will be aggregated with these of other respondents and the information you provide will not be attributed to you personally. Your participation is voluntary. Please feel free to skip any question you do not want to answer.

We would like to audio-record this interview to make sure we accurately capture everything you say. These recordings will not be shared outside of our team and will be destroyed in the end of the study.

[If using a note taker] My colleague, [name], is on the telephone with me; [he/ she] will help me take notes during the interview. Is that okay?

[If audio taping the interview]: We would like to audio-record this interview as well to make sure we accurately capture everything you say. These recordings will not be shared outside of our team and will be destroyed in the end of the study. Is that okay with you?

Do you have questions for me before we proceed?

Additional information if needed. You do not need to read:

The OMB control number for this project is 3145-0215. Public reporting burden for this collection of information is estimated to average 60 minutes per respondent, including the time for consenting. Send comments regarding this burden estimate or any other aspects of this collection of information, including suggestions for reducing this burden, to Suzanne H. Plimpton, Reports Clearance Officer, National Science Foundation, 2415 Eisenhower Ave, Alexandria, VA 22314 or send e-mail to splimpto@nsf.gov.

1. Can you tell me about your role as Managing Director, how long you have been in this role, and what brought you to it?
2. What do you see as the most important non-scientific accomplishments of the Center? To what extent have these accomplishments been made possible by the Center?
3. What programs, partnerships, and processes created by the Center do you think will remain after the funding ends?
4. In your opinion, are there certain types of problems that are better suited to the Center funding mechanism? Which of these characteristics apply to your Center?
5. Did the Center structure enable your center to more rapidly respond to scientific developments in the field? If yes, can you give some examples?
6. What are the characteristics of a successful partner and partnership? Which partnerships do you see as the most and least successful?

7. What processes, policies, and other organizational components of your Center do you see as the most effective?

8. What have been the main challenges for your Center? What would you do differently if you could start again?

9. What do you see as the main advantages and limitations of the Center model? Of the 2-phase funding mechanism?

10. In hindsight, do you think a 1-phase or 2-phase mechanism would have been more effective for your center? Should NSF maintain this mechanism for future centers?

E.5 Interviews with CCI Industry Partners

Interview Consent and OMB Notification

Thank you so much for making time today to talk with me about NSF-funded Center-based research programs. We are interviewing a sample of Principal Investigators from across NSF's center-based research community. Your feedback will inform NSF on issues relevant to the design, implementation, and evaluation of center-based research programs.

Your answers will be aggregated with these of other respondents and the information you provide will not be attributed to you personally. Your participation is voluntary. Please feel free to skip any question you do not want to answer.

We would like to audio-record this interview to make sure we accurately capture everything you say. These recordings will not be shared outside of our team and will be destroyed in the end of the study.

[If using a note taker] My colleague, [name], is on the telephone with me; [he/ she] will help me take notes during the interview. Is that okay?

[If audio taping the interview]: We would like to audio-record this interview as well to make sure we accurately capture everything you say. These recordings will not be shared outside of our team and will be destroyed in the end of the study. Is that okay with you?

Do you have questions for me before we proceed?

Additional information if needed. You do not need to read:

The OMB control number for this project is 3145-0215. Public reporting burden for this collection of information is estimated to average 20 minutes per respondent, including the time for consenting. Send comments regarding this burden estimate or any other aspects of this collection of information, including suggestions for reducing this burden, to Suzanne H. Plimpton, Reports Clearance Officer, National Science Foundation, 2415 Eisenhower Ave, Alexandria, VA 22314 or send e-mail to splimpto@nsf.gov.

1. What is the history of your partnership? When and why did you become a partner in the center? How well did you know the other participants prior to the partnership? For currently-funded CCIs]: Is the partnership still active? If not, why not?

2. What is/was the nature of your partnership? Has it changed over time?

3. For currently-funded CCIs: Do you expect the partnership to persist after the NSF funding ends? If yes, how do you envision the partnership developing?

4. In what way has your organization benefited from this partnership?

5. What do you see as the most important scientific accomplishments of the Center? Do you think they would they have been possible without the center model? If not, why not?

6. Have you experienced any challenges partnering with the Center? What were they? Have they been resolved?

7. Do you have a view about the Center organization and processes? Do you think these are effective? Are there components you would change?

E.6 Interviews with Individuals Who Have Been Involved in Oversight of CCI Centers

Interview Consent

Thank you so much for making time today to talk with me about NSF-funded Center-based research programs. We are interviewing a sample of Site Visitors and other individuals involved in oversight of CCI Centers. Your feedback will inform NSF on issues relevant to the design, implementation, and evaluation of center-based research programs.

Your answers will be aggregated with these of other respondents and the information you provide will not be attributed to you personally. Your participation is voluntary. Please feel free to skip any question you do not want to answer.

We would like to audio-record this interview to make sure we accurately capture everything you say. These recordings will not be shared outside of our team and will be destroyed in the end of the study.

[If using a note taker] My colleague, [name], is on the telephone with me; [he/ she] will help me take notes during the interview. Is that okay?

[If audio taping the interview]: We would like to audio-record this interview as well to make sure we accurately capture everything you say. These recordings will not be shared outside of our team and will be destroyed in the end of the study. Is that okay with you?

Do you have questions for me before we proceed?

1. How and how long have you been involved in the CCI Program management?
2. In what ways have the center(s) that you manage demonstrated leadership in the field and responsiveness to developments in the field?
3. How effective is the management structure of the center(s), and how well do they manage collaboration, communications, and data sharing across partners?
4. Do you think the chemistry community has benefited from CCIs? Can you give some examples of these benefits?
5. Do you expect the programs, partnerships, and processes created by the center to remain in place after the funding ends? Can you give some examples of the lasting impacts you anticipate?
6. What is your view of the 2-phase funding model? What are its advantages and disadvantages?
7. What aspects of the center evolved in unexpected ways and/or deviated from the original goals? Did these changes lead to positive outcomes?
8. Do you have similar experience with other large center similar to CCI? How do you contrast these centers to CCI? What are their relative strengths and weaknesses?
9. In your opinion, are there certain types of problems that are better suited to Center funding or that require Center funding? If so, what are the characteristics that define such problems?

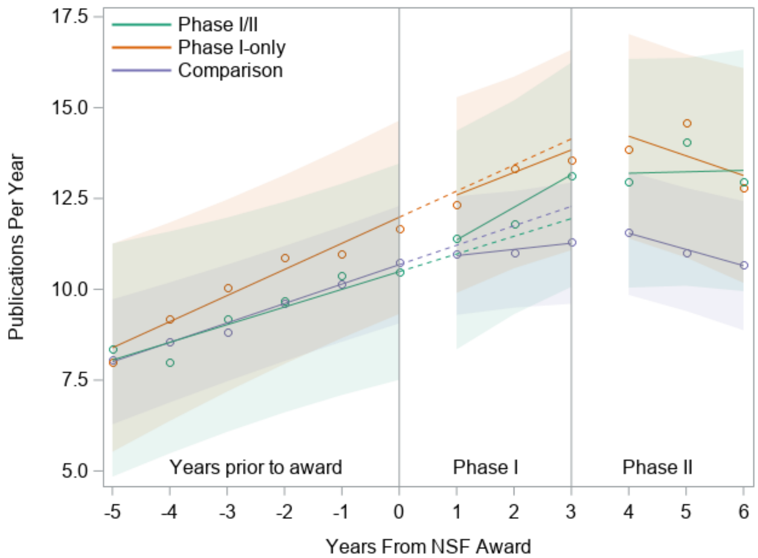
10. What do you see as the most important **scientific contributions** of the CCI center(s) you are most familiar with? The entire CCI Program, if you are able to comment? How were these accomplishments enabled by the center mechanism? Would they have been possible without the center?

11. What do you see as the most important **non-scientific contributions** of the center(s) (e.g. in workforce development, knowledge transfer, economic benefits, or educating the general public)? How were these accomplishments enabled by the center mechanism? Would they have been possible without the center?

Appendix F: Sensitivity Analyses

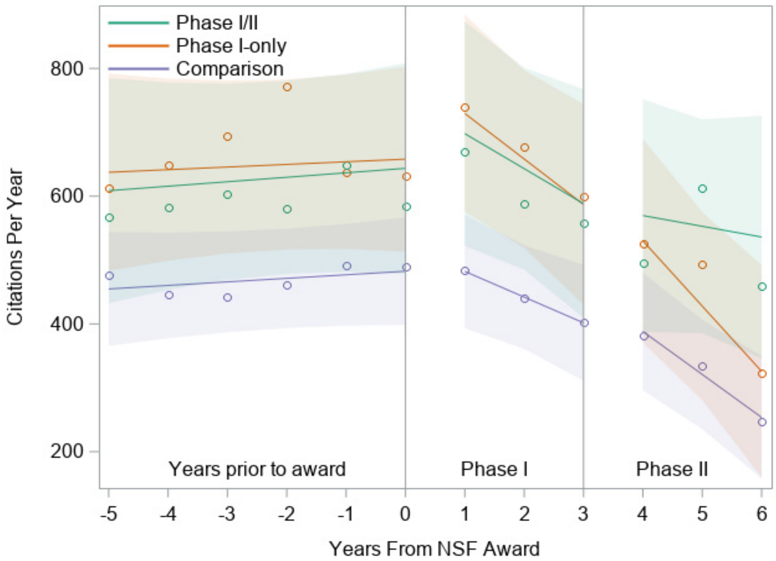
This appendix contains sensitivity analyses for the comparative short interrupted time series (C-SITS) models presented in the main report. Investigators with number of publications in the top one percentile of the sample (more than 93 in a year) were excluded from the primary analysis, given the high probability that their data inadvertently combines publications from multiple individuals with the same name. The sensitivity analyses with the full sample (including the top percentile) are presented here. Differences in statistical significance from the primary analyses are noted. In general, standard errors in the sensitivity analyses are larger than those in the primary analyses, so differences between groups are less likely to be statistically significant.

Exhibit F-1: Publications



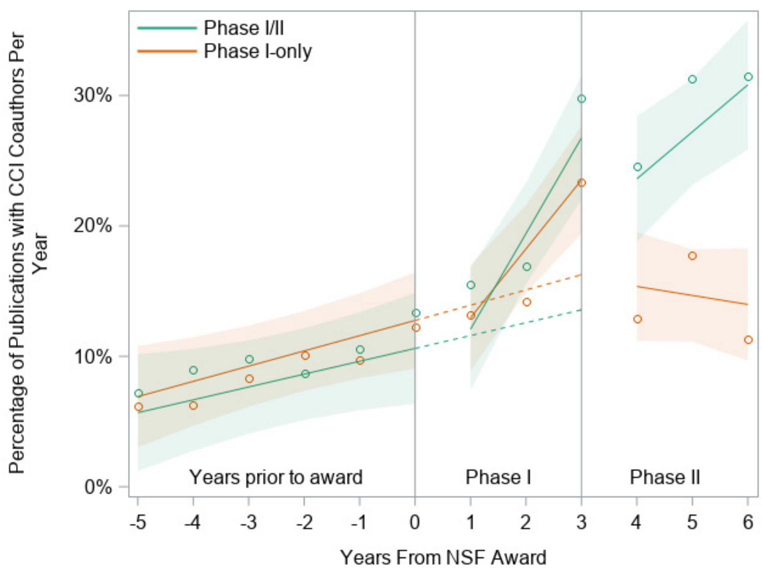
None of the significant differences highlighted in the primary report model for publications hold in the sensitivity analysis.

Exhibit F-2: Citations



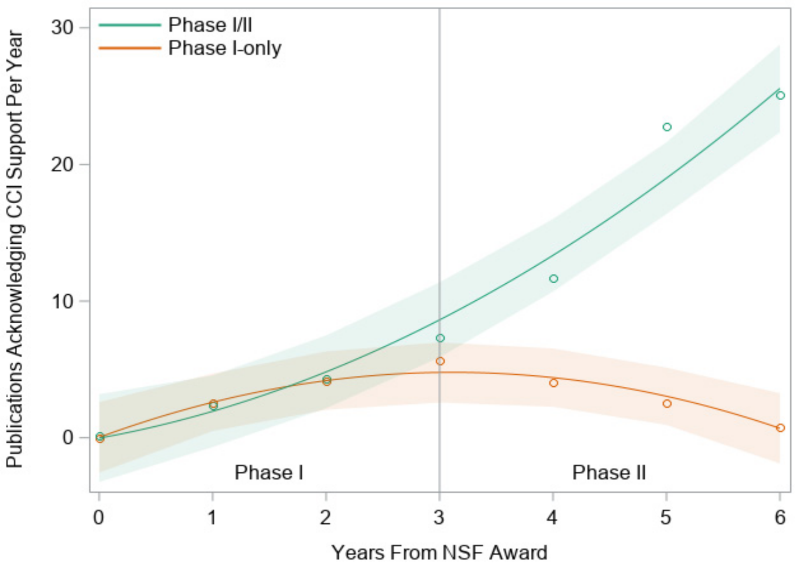
At Center Year 0, Phase I-only investigators have significantly more citations that comparison investigators (Phase I/II investigators do not).

Exhibit F-3: Co-authorship



There are no differences in statistical significance from the primary model presented in the main report (investigators with high publication counts did not have unusual co-authorship rates).

Exhibit F-4: Publications Acknowledging CCI



This sensitivity analysis fits a single quadratic model to each group rather than an interrupted linear model. In this model, there is a significant difference between Phase I and II at Center Year 3 (7 versus 5, $p < .05$).

Appendix G: Grand Challenges

G.1 Grand Challenges in Chemistry

Scientific American October 2011 "10 Unsolved Mysteries in Chemistry"

- Chemical origins of life
- The nature of the chemical bond (chemical modeling)
- Carbon nanotechnology
- Artificial photosynthesis
- Devising catalysts for biofuels
- Understanding chemical basis for thought and memory
- Understanding the chemical basis for epigenetics
- Finding new ways to make complex molecules
- Integrating chemistry: creating a chemical information technology
- New forms of matter, periodic table

The National Academies Press "Chemistry Future"

- Synthesize and manufacture any new substance (synthesis process should be highly selective, low energy, and environmentally benign)
- Understand and control how molecules react
- Understand the chemistry of living systems in detail
- Pharma
- Develop self-assembly capabilities
- Understand complex chemistry of the earth
- Sustainable and inexpensive energy

American Chemical Society 2016 Editorial

- Using genetic information to understand the molecular basis of disease – to help in the development of new treatments and preventative strategies
- Sustainable energy, light harvesting
- Pollution prevention/treatment
- Resource efficiency
- Computational chemistry to understand complex systems
- Understanding the chemical bond

G.2 Societal Grand Challenges

European Union Horizon 2020

- Health, demographic change and well-being
- Food security, sustainable agriculture and forestry, marine, maritime and inland water research, and the bioeconomy
- Secure, clean and efficient energy
- Smart, green and integrated transport
- Climate action, environment, resources efficiency and raw materials
- Inclusive, innovative and reflective societies
- Secure societies – protecting freedom

United Nations Sustainable Development Goals

- End poverty in all forms
- End hunger, achieve food security and improved nutrition, promote sustainable agriculture
- Ensure healthy lives and promote well-being for all
- Ensure inclusive and equitable quality education
- Achieve gender equality
- Ensure availability and sustainable management of water and sanitation for all
- Ensure access to affordable, reliable, sustainable, and clean energy for all
- Promote sustained, inclusive, sustainable economic growth
- Build resilient infrastructure, promote inclusive and sustainable industrialization
- Reduce inequality
- Sustainable Cities
- Ensure sustainable consumption and production
- Take urgent action to combat climate change
- Sustainable use of marine resources
- Sustainable use of terrestrial resources
- Promote peace

Appendix H: Supplemental Survey Tables from PIs/Co-Investigators

This section contains supplemental exhibits for all PI/Co-Investigator survey questions that are presented in the report exhibits. The supplemental exhibits present estimated percentages measured on complete categorical scales (e.g., strongly agree to strongly disagree). Percentages for survey item response options may differ between the report exhibits and the supplemental exhibits because the study team excluded respondents who selected Don't Know or Not Applicable from the denominator in the report exhibits only. Tables that match report exhibits can be found in Appendix J.

Exhibit H-1: Time Associated with CCI

	Phase I	Phase II	Overall
6 or fewer months	0%	0%	0%
7 to 11 months	0%	0%	0%
1 year	0%	2%	2%
2 to 4 years	94%	18%	27%
5 to 6 years	0%	23%	20%
7 or more years	0%	54%	48%
Uncertain/do not recall	6%	3%	3%

Note: Phase I (N = 18, missing = 0), Phase II (N = 116, missing = 0), overall (N = 134, missing = 0).

Source: Survey of Principal Investigators and Co-Investigators Q3 (For how long have you been or were you associated with the CCI Program?).

Exhibit H-2: CCI Research Characteristics

	n	Not at All	To Some Extent	To a Considerable Extent
Addresses important societal problem	133	6%	29%	65%
Focuses on major scientific challenge(s) in fundamental chemistry	134	2%	1%	97%
Has the potential to radically change our understanding of an important scientific or engineering concept	134	2%	10%	88%
Interdisciplinary	134	1%	16%	83%
High-risk	134	4%	29%	67%
Requires a coordinated effort from diverse experts	134	0%	10%	90%
Requires large investment of funds	134	1%	17%	82%

Note: N = 134, missing = 0–1.

Source: Survey of Principal Investigators and Co-Investigators Q4 (To what extent does the research conducted by your CCI have the following characteristics?).

Exhibit H-3: CCI Partner Collaboration Prior to Center Establishment

	Percent
None of the partners	42%
Some of the partners	54%
Half or more of the partners	4%

Note: N = 134, missing = 1.

Source: Survey of Principal Investigators and Co-Investigators Q5 (Had you collaborated with any or all of the CCI partners before the center was established?).

Exhibit H-4: Extent of Changes in Collaboration

	Percent
Not at all	2%
To some extent	32%
To a considerable extent	66%

Note: N = 77, missing = 0

Limited to respondents who collaborated with at least some of the CCI partners before the center was established.

Source: Survey of Principal Investigators and Co-Investigators Q6 (Has the nature and/or extent of these collaborations changed because of CCI participation?)

Exhibit H-4a: Continuation of Collaboration

	Percent
No	9%
I expect to maintain some CCI collaborations after the grant ends	71%
I expect to maintain most or all CCI collaborations after the grant ends	13%
Uncertain	7%

Note: N = 134, Missing = 2

Source: Survey of Principal Investigators and Co-Investigators Q7 (Do you expect to continue collaborating with CCI partners after grant ends?)

Exhibit H-5: Benefits of CCI Participation

	n	No Benefit Due to CCI	Some Benefit Due to CCI	Large Benefit Due to CCI	Not Applicable
At Lead Institution					
Ability to attract better qualified or more diverse students and postdocs to your research group	52	10%	26%	60%	3%
Ability to generate new and/or better ideas	53	8%	12%	76%	4%
Ability to more quickly/effectively respond to scientific developments	53	10%	29%	56%	6%
Ability to obtain additional funding to support your research	53	16%	40%	37%	7%
Ability to take your research in a new direction	52	10%	6%	80%	5%
Access to resources at partner institutions	53	17%	42%	37%	4%
Access to resources at your institution	53	9%	36%	48%	7%
Use of new theoretical models	53	13%	37%	37%	13%
Use of new/additional data sources	53	11%	34%	39%	16%
Use of new/additional instrumentation or technology	53	9%	19%	63%	9%
Use of new/additional theoretical or experimental models	53	12%	27%	52%	9%
Not at Lead Institution					
Ability to attract better qualified or more diverse students and postdocs to your research group	82	5%	37%	53%	4%
Ability to generate new and/or better ideas	82	1%	23%	75%	1%
Ability to more quickly/effectively respond to scientific developments	82	5%	37%	57%	1%
Ability to obtain additional funding to support your	82	13%	44%	38%	4%

	n	No Benefit Due to CCI	Some Benefit Due to CCI	Large Benefit Due to CCI	Not Applicable
research					
Ability to take your research in a new direction	82	0%	18%	79%	3%
Access to resources at partner institutions	81	1%	38%	59%	1%
Access to resources at your institution	82	43%	32%	21%	4%
Use of new theoretical models	82	10%	41%	41%	7%
Use of new/additional data sources	82	12%	35%	43%	10%
Use of new/additional instrumentation or technology	82	7%	45%	39%	10%
Use of new/additional theoretical or experimental models	82	5%	31%	56%	8%
Overall					
Ability to attract better qualified or more diverse students and postdocs to your research group	136	7%	33%	56%	4%
Ability to generate new and/or better ideas	137	4%	18%	75%	2%
Ability to more quickly/effectively respond to scientific developments	137	7%	34%	56%	3%
Ability to obtain additional funding to support your research	137	14%	43%	38%	5%
Ability to take your research in a new direction	136	4%	13%	79%	4%
Access to resources at partner institutions	136	7%	40%	50%	3%
Access to resources at your institution	137	30%	34%	31%	5%
Use of new theoretical models	137	12%	40%	39%	9%
Use of new/additional data sources	137	12%	35%	41%	12%
Use of new/additional instrumentation or technology	137	8%	35%	48%	9%
Use of new/additional theoretical or experimental models	137	8%	30%	55%	8%

Note: Not at Lead Institution (N = 82, Missing = 0-1); At Lead Institution (N = 52, Missing = 0-1); Overall (N = 134, Missing = 0-1);

Source: Survey of Principal Investigators and Co-Investigators Q8 (Please indicate whether participation in the CCI has benefited your research program.)

Exhibit H-6: Perceived Effect of CCI on Publication Patterns, Research Interests, and/or Professional Visibility

	n	Increased Due to CCI Participa-tion	Increased, but Not Due to CCI Participa-tion	Has Not Changed / Too Early to Tell	Decreased Due to CCI Participa-tion	Decreased, but Not Due to CCI Participa-tion
Number of papers published per year	128	65%	7%	21%	3%	4%
Journal quality	129	43%	8%	48%	0%	1%
Range of journals	126	45%	10%	43%	1%	1%
Publishing with industry	129	13%	8%	75%	1%	3%
Funding from industry	129	15%	9%	72%	1%	3%
Interest in commercialization	129	31%	7%	61%	1%	0%
Participation in new professional conferences, associations or societies	129	50%	5%	43%	1%	1%
Number of speaking invitations	129	47%	17%	33%	1%	2%
Requests to serve on dissertation committees outside your home institution	128	15%	9%	75%	1%	1%
Requests to serve on advisory panels	129	31%	8%	59%	1%	1%
Requests to serve on editorial board of journals	129	12%	10%	76%	1%	1%
Requests to serve as a peer reviewer	129	43%	15%	40%	2%	0%
Requests to provide policy advice or testimony	127	9%	5%	85%	1%	1%
Receipt of awards, fellowships, or chaired positions	129	28%	9%	62%	1%	0%
Diversity of research problems on which you work	129	75%	13%	11%	1%	0%

Note: N = 134, Missing = 5-8

Source: Survey of Principal Investigators and Co-Investigators Q9 (Have any of the following changes occurred in your publication patterns, research interests, and/or professional visibility since you began participating in CCI?)

Exhibit H-7: Resources Created or Improved by CCI

	Percent
Methods	83%
Educational or outreach materials	79%
Lessons learned for how to run a large center	77%
New partnerships	75%
Communication infrastructure	57%
Data	57%
Equipment	51%
Facilities	43%
Data management system	39%
Reagents	36%
Other resources, please specify	2%

Note: N = 134, Missing = 0

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q10 (Which of the following resources have been created or improved by CCI?)

Exhibit H-7a: Resources Used by Unaffiliated Researchers

	Percent
Methods	73%
Educational or outreach materials	70%
Facilities	69%
Equipment	66%
Reagents	61%
Data	60%
Lessons learned for how to run a large center	45%
New partnerships	43%
Data management system	27%
Communication infrastructure	26%
Other resources, please specify	69%

Note: N=111, missing = 0

Each row is limited to respondents who indicated the resource was created or improved by CCI in Q10.

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q10A (Which of these resources, if any, are being used by researchers not affiliated with the center?)

Exhibit H-8: Educational and/or Outreach Opportunities Developed or Improved by CCI

	Percent
Research and teaching experiences for students and postdocs	88%
Programs for educating the public about chemistry	86%
Mechanisms for recruitment and/or retention of individuals from underrepresented groups	74%
Mechanisms for mentorship of individuals from underrepresented groups	68%
Engagement with organizations focused on outreach and advocacy to pre-college, public, or policymaker audiences	64%
Engagement with organizations with expertise supporting underrepresented groups in the scientific community	63%
Courses/seminars in chemistry	63%
Training programs in chemistry	61%
I do not know whether my CCI developed or improved these types of opportunities	7%

Note: N=134, missing = 0

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q11 (Please indicate whether your CCI developed or improved the following educational and/or outreach opportunities.)

Exhibit H-9: Educational and/or Outreach Opportunities Expected to be Sustained after Grant End

	Percent
Research and teaching experiences for students and postdocs	70%
Courses/seminars in chemistry	69%
Mechanisms for mentorship of individuals from underrepresented groups	65%
Programs for educating the public about chemistry	64%
Engagement with organizations with expertise supporting underrepresented groups in the scientific community	61%
Mechanisms for recruitment and/or retention of individuals from underrepresented groups	58%
Training programs in chemistry	47%
Engagement with organizations focused on outreach and advocacy to pre-college, public, or policymaker audiences	44%

Note: N=117, missing = 0

Each row is limited to respondents who indicated that the opportunity was developed or improved by their CCI in Q11.

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q12 (Please indicate whether you expect to be able to sustain the following programs and activities after the grant ends If your grant has ended, please indicate whether these programs and activities are still in place.)

Exhibit H-10: Improvements Due to CCI

	n	No Improvement Due to CCI	Some Improvement Due to CCI	Large Improvement Due to CCI	N/A
Increased participation of underrepresented groups in your lab	130	21%	58%	16%	5%
Increased participation of underrepresented groups at your institution	130	33%	51%	6%	11%
Improved ability of students and postdocs to obtain a position after leaving CCI	130	14%	36%	43%	6%
Improved quality of education in chemistry	130	16%	53%	25%	5%
Increased interest in/understanding of chemistry among the public you were able to reach	128	12%	43%	39%	5%

Note: N=134, missing = 4-6

Source: Survey of Principal Investigators and Co-Investigators Q13 (Please indicate whether the following improvements have occurred as a result of CCI funding)

Exhibit H-11: Industry Benefits Due to CCI

	n	No Benefit Due to CCI	Some Benefit Due to CCI	Large Benefit Due to CCI	Uncertain
New or improved ideas for commercial product or process	129	14%	40%	32%	14%
New or improved product or process	129	17%	38%	28%	16%
Reduction in environmental impact	126	21%	30%	21%	28%
Ability to meet regulatory requirements	126	33%	17%	3%	47%
Access to personnel	126	11%	28%	42%	18%
Increase in sales	124	34%	6%	1%	59%
Cost savings	122	31%	11%	3%	55%

Note: N=134, missing = 5-12

Source: Survey of Principal Investigators and Co-Investigators Q14 (Please indicate whether the CCI delivered any of the following benefits to industry.)

Exhibit H-12: Satisfaction with Various Elements of CCI

	n	N/A	Very Dissatisfied	Dissatisfied	Neutral	Satisfied	Very Satisfied
At Lead Institution							
Requirement to develop a strategic plan	50	3%	3%	7%	17%	40%	30%
Distribution of resources among partners	50	2%	7%	7%	16%	29%	40%
Sharing of credit among partners	50	0%	7%	3%	10%	41%	39%
Intellectual contribution of partners	50	0%	5%	4%	5%	36%	49%
Productivity of meetings among partners	50	3%	4%	4%	17%	42%	30%
Frequency of meeting among partners	50	0%	3%	10%	12%	38%	37%
Communication tools	50	0%	5%	6%	7%	52%	30%
Data sharing tools	50	3%	3%	6%	20%	41%	28%
Professional development opportunities for students/postdocs	50	3%	8%	1%	3%	26%	58%
Broadening participation activities and programs	50	3%	5%	0%	9%	24%	58%
Public outreach activities and programs	50	3%	3%	1%	6%	17%	70%
Leadership of the center	50	6%	10%	3%	7%	18%	57%
Overall direction of the center	50	3%	12%	1%	1%	28%	54%
Funding level for Phase I	50	9%	8%	8%	6%	33%	36%
Duration of Phase I	50	9%	8%	4%	6%	38%	34%
Funding level for Phase II	41	4%	3%	0%	7%	19%	67%
Duration of Phase II	41	7%	3%	0%	7%	21%	62%
Not at Lead Institution							
Requirement to develop a strategic plan	78	5%	2%	1%	18%	50%	24%
Distribution of resources among partners	79	2%	5%	9%	6%	38%	40%
Sharing of credit among partners	80	2%	3%	6%	6%	36%	46%
Intellectual contribution of partners	80	3%	2%	4%	4%	35%	52%
Productivity of meetings among partners	80	2%	2%	3%	6%	48%	39%
Frequency of meeting among partners	80	2%	3%	3%	8%	52%	31%
Communication tools	79	2%	3%	1%	11%	44%	38%
Data sharing tools	79	4%	2%	1%	31%	44%	17%
Professional development opportunities for students/postdocs	80	1%	2%	1%	4%	31%	61%
Broadening participation activities and programs	80	3%	2%	0%	6%	25%	64%
Public outreach activities and programs	80	1%	3%	2%	2%	33%	58%

	n	N/A	Very Dissatisfied	Dissatisfied	Neutral	Satisfied	Very Satisfied
Leadership of the center	80	1%	5%	0%	6%	23%	66%
Overall direction of the center	80	1%	3%	1%	8%	24%	63%
Funding level for Phase I	80	41%	2%	3%	13%	25%	16%
Duration of Phase I	79	39%	1%	1%	15%	25%	19%
Funding level for Phase II	72	6%	4%	2%	4%	41%	43%
Duration of Phase II	73	8%	4%	2%	7%	37%	42%
Overall							
Requirement to develop a strategic plan	130	4%	2%	3%	17%	46%	26%
Distribution of resources among partners	131	2%	6%	8%	10%	34%	40%
Sharing of credit among partners	132	1%	5%	5%	8%	38%	43%
Intellectual contribution of partners	132	2%	3%	4%	5%	35%	51%
Productivity of meetings among partners	132	3%	3%	4%	10%	45%	35%
Frequency of meeting among partners	132	1%	3%	6%	10%	47%	33%
Communication tools	131	1%	4%	3%	10%	47%	35%
Data sharing tools	131	3%	2%	3%	27%	43%	21%
Professional development opportunities for students/postdocs	132	2%	4%	1%	3%	29%	60%
Broadening participation activities and programs	132	3%	3%	0%	7%	25%	62%
Public outreach activities and programs	132	2%	3%	2%	4%	27%	63%
Leadership of the center	132	3%	7%	1%	6%	21%	62%
Overall direction of the center	132	2%	6%	1%	5%	25%	59%
Funding level for Phase I	132	29%	4%	5%	10%	28%	24%
Duration of Phase I	131	28%	4%	2%	11%	30%	25%
Funding level for Phase II	115	5%	4%	1%	5%	33%	52%
Duration of Phase II	116	8%	4%	1%	7%	31%	49%

Note: Not at Lead Institution (N = 82, missing = 2-10); At Lead Institution (N = 52, missing = 3-12); Overall (N = 134, missing = 5-22)

Source: Survey of Principal Investigators and Co-Investigators Q15 (How satisfied are you with the following elements of CCI?)

Exhibit H-13: Contributions to Center Success

	n	Not at All	To Some Extent	To a Considerable Extent
At Lead Institution				
Overall direction of the center	42	0%	14%	86%
Leadership of the center	41	0%	15%	85%
Duration of Phase II	38	4%	15%	81%
Funding level for Phase II	39	3%	23%	74%
Intellectual contribution of partners	45	2%	28%	70%
Public outreach activities and programs	46	6%	30%	64%
Professional development opportunities for students/postdocs	44	0%	37%	63%
Broadening participation activities and programs	46	3%	35%	62%
Productivity of meetings among partners	45	2%	38%	61%
Sharing of credit among partners	44	5%	36%	59%
Frequency of meeting among partners	44	2%	42%	57%
Funding level for Phase I	37	4%	40%	56%
Distribution of resources among partners	42	3%	44%	52%
Duration of Phase I	39	3%	45%	51%
Communication tools	44	4%	46%	51%
Requirement to develop a strategic plan	44	3%	48%	49%
Data sharing tools	43	5%	66%	28%
Not at Lead Institution				
Leadership of the center	74	1%	18%	81%
Duration of Phase II	62	0%	20%	80%
Overall direction of the center	74	0%	20%	80%
Funding level for Phase II	61	0%	22%	78%
Intellectual contribution of partners	72	0%	24%	76%
Professional development opportunities for students/postdocs	75	1%	33%	66%
Distribution of resources among partners	65	0%	38%	62%
Productivity of meetings among partners	73	0%	40%	60%
Sharing of credit among partners	70	1%	41%	58%
Public outreach activities and programs	74	2%	44%	54%
Broadening participation activities and programs	75	2%	45%	53%
Communication tools	72	4%	49%	46%
Requirement to develop a strategic plan	69	4%	52%	44%
Funding level for Phase I	40	5%	51%	44%
Duration of Phase I	46	6%	53%	41%
Frequency of meeting among partners	71	0%	59%	41%
Data sharing tools	71	24%	52%	24%

	n	Not at All	To Some Extent	To a Considerable Extent
Overall				
Leadership of the center	117	1%	17%	82%
Overall direction of the center	118	0%	18%	82%
Duration of Phase II	102	1%	18%	80%
Funding level for Phase II	102	1%	22%	76%
Intellectual contribution of partners	119	1%	25%	74%
Professional development opportunities for students/postdocs	121	1%	35%	65%
Productivity of meetings among partners	120	1%	39%	60%
Distribution of resources among partners	109	1%	40%	58%
Sharing of credit among partners	116	2%	39%	58%
Public outreach activities and programs	122	4%	39%	58%
Broadening participation activities and programs	123	3%	41%	56%
Funding level for Phase I	79	4%	46%	50%
Communication tools	118	4%	48%	48%
Frequency of meeting among partners	117	1%	53%	47%
Requirement to develop a strategic plan	115	4%	50%	46%
Duration of Phase I	87	5%	49%	46%
Data sharing tools	116	17%	57%	26%

Note: Not at Lead Institution (N = 40-50, missing = 3-12); Overall (N = 85-127, missing = 6-24);

Each row is limited to respondents who were not dissatisfied with the element, according to Q15.

Source: Survey of Principal Investigators and Co-Investigators Q16 (To what extent have these elements contributed to the success of your center?)

Exhibit H-14: Overall Experience with CCI

	Percent
Very satisfied	60%
Satisfied	26%
Neutral	5%
Dissatisfied	3%
Very dissatisfied	6%

Note: N = 134, missing = 6

Source: Survey of Principal Investigators and Co-Investigators Q17 (Overall, how would you rate your experience in the CCI?)

Exhibit H-15: Challenges Experienced

	Percent
Technical or experimental challenges	58%
Terminating unsuccessful projects	42%
Coordination of activities between partners	40%
Communication between partners	38%
Delays in progress of research	33%
Meeting administrative requirements	31%
Contributions by partners to the center	25%
Sharing of credit for discovery	21%
Staffing of the center	21%
Seeding new projects	18%
Access to needed resources	17%
Other challenge, please specify	6%

Note: N = 134, missing = 0

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q18 (Has your CCI experienced the following challenges?)

Exhibit H-16: Extent of Challenge Resolution

	n	Not at All	To Some Extent	To a Considerable Extent
Technical or experimental challenges	78	2%	43%	56%
Terminating unsuccessful projects	56	6%	41%	53%
Coordination of activities between partners	55	5%	60%	35%
Communication between partners	49	7%	51%	42%
Delays in progress of research	46	5%	54%	41%
Meeting administrative requirements	41	5%	49%	46%
Contributions by partners to the center	33	8%	50%	42%
Sharing of credit for discovery	27	18%	51%	31%
Staffing of the center	27	3%	58%	40%
Access to needed resources	20	9%	54%	37%
Seeding new projects	24	3%	46%	50%
Other challenge, please specify	6	79%	0%	21%

Note: N = 79, missing = 0-3

Each row is limited to respondents who indicated that the challenge had been experienced, according to Q18.

Source: Survey of Principal Investigators and Co-Investigators Q19 (To what extent have these challenges been resolved?)

Exhibit H-17: Phase I Participation Contribution to Success of Phase II Center

	Percent
Not at all	2%
To some extent	7%
To a considerable extent	51%
I did not participate in Phase I	40%

Note: N = 116, missing = 5

Source: Survey of Principal Investigators and Co-Investigators Q20 (To what extent has participation in Phase I contributed to the success of your Phase II center?)

Exhibit H-18: Results of Participation in Phase I

	Percent
Formed new or cemented old collaborations	80%
Advanced your research program	75%
Provided training or career development opportunities for students or postdocs	73%
New direction for your research program	71%
Gained experience of participating in or running a center	67%
Developed educational or public outreach programs	56%
Developed center policies and procedures	46%
Obtained additional funding to support your research	45%
No benefits of participation in Phase I	3%
Other benefits, please describe	3%

Note: N = 92, missing = 4

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q21 (Have any of the following occurred as a result of your participation in Phase I?)

Exhibit H-19: Ability to Continue Working on CCI Funded Projects after Grant End

	Percent
Yes	76%
No	24%

Note: N = 18, missing = 2

Limited to Phase I respondents

Source: Survey of Principal Investigators and Co-Investigators Q22 (Were you able to continue working on the projects that had been funded by CCI after the grant ended?)

Exhibit H-20: Advantages of 2-Phase Model

	Phase I	Phase II	Overall
It allows the centers to refine their research goals and approach	58%	86%	83%
It enables selection of better Phase II centers by NSF	28%	75%	69%
It allows the centers to pilot activities and programs	62%	67%	67%
It allows selection of the right partners	54%	67%	65%
It allows the centers to develop and test policies and procedures	28%	54%	51%
It allows participants to determine whether they like the experience	19%	40%	37%
No advantages	17%	5%	6%
Other advantages, please specify	0%	2%	2%

Note: Phase I (N = 18, missing = 2); Phase II (N = 116, missing = 2); Overall (N = 134, missing = 4);

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q23 (In your view, which of the following are the advantages of the 2-phase model?)

Exhibit H-21: Disadvantages of 2-Phase Model

	Phase I	Phase II	Overall
Some strong applicants may be discouraged from applying	26%	17%	18%
Insufficient resources for Phase I grantees not selected for Phase II to continue their research	79%	33%	39%
Time burden to submit a Phase II application	51%	35%	36%
Delay in tacking time-sensitive topics	0%	12%	10%
No disadvantages	0%	24%	21%
Other disadvantages, please specify	36%	8%	11%

Note: Phase I (N = 18, missing = 2); Phase II (N = 116, missing = 2); Overall (N = 134, missing = 4);

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q24 (In your view, what are the disadvantages of the 2-phase model?)

Exhibit H-22: Preference for 2-Phase Model to Single Phase

	Phase I	Phase II	Overall
Yes, 2-phase model is preferable	43%	80%	76%
No, 1-phase model is preferable	38%	6%	9%
Uncertain	19%	15%	15%

Note: Phase I (N = 18, missing = 3); Phase II (N = 116, missing = 3); Overall (N = 134, missing = 6);

Source: Survey of Principal Investigators and Co-Investigators Q25 (On balance, is a 2-phase center model preferable to a single phase?)

Appendix I: Supplemental Survey Tables from Graduate Students/Postdocs

This section contains supplemental exhibits for all Graduate Student/Postdoc survey questions that are presented in the report exhibits. The supplemental exhibits present estimated percentages measured on complete categorical scales (e.g., strongly agree to strongly disagree). Percentages for survey item response options may differ between the report exhibits and the supplemental exhibits because the study team excluded respondents who selected Don’t Know or Not Applicable from the denominator in the report exhibits only. Tables that match report exhibits can be found in Appendix J.

Exhibit I-1: Time in CCI

	Percent
3 or fewer months	0%
4 to 6 months	2%
7 to 11 months	3%
1 year	10%
2 to 3 years	50%
4 or more years	33%
Uncertain/do not recall	2%

Note: N = 340, missing = 0

Source: Survey of Current and Former Graduate Students and Postdocs Q4 (For how long have you been associated with the CCI Program?)

Exhibit I-2: Reason for Leaving

	Percent
Graduated/completed postdoctoral training	87%
Left for another reason	13%

Note: N = 240, missing = 0

Limited to past students.

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Current and Former Graduate Students and Postdocs Q5 (Why are you no longer participating in CCI?)

Exhibit I-2a: Other Reasons for Leaving CCI

	Percent
Completed CCI-related project and moved on to a project not related to CCI	38%
Decided to pursue another career path	18%
Advisor left the CCI	10%
Did not get along with advisor/inadequate mentoring	10%
Left graduate/postdoctoral program before completion	9%
Was assigned to a different project	9%
Personal/family reason or change in life circumstances	8%
Insufficient funding	5%
Did not get resources I needed	4%
Was not interested in research being conducted	2%
Did not get along with people in the center	0%
Did not like being part of a center	0%
Other, please explain	17%

Note: N = 34, missing = 0

Limited to students no longer participating in CCI for a reason other than completing their postdoctoral training.

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Current and Former Graduate Students and Postdocs Q5A (Please indicate all reasons [for leaving] that apply)

Exhibit I-3: Student Type

	Percent
A terminal masters student	2%
A doctoral student	62%
A postdoctoral scholar	35%
Other, please explain	0%

Note: N = 340, missing = 0

Source: Survey of Current and Former Graduate Students and Postdocs Q6 (During your final year at CCI, are you:)

Exhibit I-4: Number of Mentors

	Graduate	Postdoc	Overall
I have a single mentor who participates in CCI	38%	49%	42%
I have a single mentor who does not participate in CCI	2%	0%	2%
I have multiple mentors who all participate in CCI	35%	41%	37%
I have multiple mentors, but not all of them participate in CCI	23%	10%	19%
I do not have any mentors	1%	1%	1%

Note: Graduate (N = 227, missing = 0); Postdoc (N = 113, missing = 0); Overall (N = 340, missing = 0);

Source: Survey of Current and Former Graduate Students and Postdocs Q7 (How many people served as mentors to you (either formally or informally), providing guidance, feedback, and support for your development and research?)

Exhibit I-5: Influence of CCI on Various Choices

	Graduate	Postdoc	Overall
Type of institution to join – e.g., university, industry, government	43%	39%	41%
Type of career to pursue – e.g., research, teaching, entrepreneurship	55%	52%	54%
Whether to pursue a doctoral or professional degree	2%	0%	1%
Whether to pursue postdoctoral training	42%	9%	28%
Choice of specific employer	13%	10%	12%
Choice of discipline/field of study	33%	36%	34%
Choice of research problem	37%	50%	42%
Choice of advisor/mentor	25%	16%	21%
None of the above	0%	0%	0%

Note: Graduate (N = 145, missing = 0); Postdoc (N = 95, missing = 0); Overall (N = 240, missing = 0).

Limited to past students.

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Current and Former Graduate Students and Postdocs Q8 (Did your CCI experiences influence any of these choices?)

Exhibit I-6: Currently Enrolled in Degree Program

	Percent
Yes	8%
No	92%

Note: N = 240, missing = 1

Limited to past students.

Source: Survey of Current and Former Graduate Students and Postdocs Q9 (Are you currently enrolled in a degree program?)

Exhibit I-6a: Degree in Chemistry or Related Field

	Graduate	Postdoc	Overall
Yes	95%	100%	95%
No	5%	0%	5%

Note: Graduate (N = 18, missing = 0); Postdoc (N = 1, missing = 0); Overall (N = 19, missing = 0);

Limited to past students currently enrolled in a degree program.

Source: Survey of Current and Former Graduate Students and Postdocs Q9A (Is your degree program in chemistry or a related field?)

Exhibit I-7: Type of Principal Employer

	Graduate	Postdoc	Overall
Not employed	4%	0%	2%
Entrepreneur/self-employed	2%	1%	2%
K-12 school or district	0%	0%	0%
Research institution/think tank	3%	4%	4%
Non-government lab	1%	3%	1%
Government (including government research labs)	14%	9%	12%
Industry (chemical or pharmaceutical company or similar)	36%	20%	29%
College or university	32%	60%	44%
Other, please specify	7%	3%	5%
Other nonprofit organization or private foundation	2%	0%	1%

Note: N = 220, missing = 0

Limited to past students not currently enrolled in a degree program

Source: Survey of Current and Former Graduate Students and Postdocs Q10 (Which of the following best describes your current principal employer?)

Exhibit I-8: Interest in Pursuing Post-Degree Positions

	n	Never Been My Goal	Considered before Involvement in CCI	Became a Goal since Involvement in CCI
Graduate Student				
Program officer/academic administrator	76	86%	7%	7%
Non-tenure-track researcher in a university or a research institute	77	66%	25%	10%
Business position in industry or an entrepreneur	77	65%	15%	21%
Science policy, law, consulting, or science writing	76	54%	18%	28%
Faculty member in a 2-year or 4-year teaching college	77	48%	41%	11%
Researcher in a government laboratory	78	35%	34%	31%
Faculty member in a research college or university	81	33%	57%	10%
Research and development position in industry	78	11%	56%	33%
Postdoc				
Business position in industry or an entrepreneur	16	81%	13%	5%
Science policy, law, consulting, or science writing	16	79%	21%	0%
Program officer/academic administrator	16	73%	15%	11%
Non-tenure-track researcher in a university or a research institute	16	71%	15%	13%
Faculty member in a 2-year or 4-year teaching college	16	55%	38%	8%
Researcher in a government laboratory	16	35%	46%	19%
Research and development position in industry	16	30%	48%	22%
Faculty member in a research college or university	18	3%	80%	17%
Overall				
Program officer/academic administrator	92	83%	9%	8%
Business position in industry or an entrepreneur	93	68%	15%	18%
Non-tenure-track researcher in a university or a research institute	93	67%	23%	10%
Science policy, law, consulting, or science writing	92	59%	18%	22%
Faculty member in a 2-year or 4-year teaching college	93	50%	40%	10%
Researcher in a government laboratory	94	35%	36%	29%
Faculty member in a research college or university	99	26%	62%	12%
Research and development position in industry	94	15%	54%	31%

Note: Graduate Student (N = 82, missing = 0-6); Postdoc (N = 18, missing = 0-2); Overall (N = 100, missing = 1-8).

Limited to current students.

Source: Survey of Current and Former Graduate Students and Postdocs Q11 (Which of the following positions are you most interested in pursuing after you complete your degree and/or postdoctoral training? Have your career goals changed since you began participating in the CCI?)

Exhibit I-9: Time Spent with Other CCI Partner

	Center for Aerosol Impacts on Climate and the Environ-ment	Center for Chemical Evolution	Center for Chemical Innovation in Solar Fuels	Center for Enabling New Tech-nologies through Catalysis	Center for Selective C-H Functional-ization	Center for Sustainable Materials Chemistry	Center for Sustainable Nano-technology	Center for Sustainable Polymers	Center for Chemistry at the Space-Time Limit	Over-all
Yes	31%	17%	24%	9%	27%	21%	57%	12%	8%	23%
No	69%	83%	76%	91%	73%	79%	43%	88%	92%	77%

Note: Center for Aerosol Impacts on Climate and the Environment (N = 31, missing = 0); Center for Chemical Evolution (N = 23, missing = 0); Center for Chemical Innovation in Solar Fuels (N = 29, missing = 1); Center for Enabling New Technologies through Catalysis (N = 54, missing = 0); Center for Selective C-H Functionalization (N = 47, missing = 0); Center for Sustainable Materials Chemistry (N = 43, missing = 0); Center for Sustainable Nanotechnology (N = 49, missing = 0); Center for Sustainable Polymers (N = 41, missing = 0); Center for Chemistry at the Space-Time Limit (N = 23, missing = 0); Overall (N = 340, missing = 1);

Source: Survey of Current and Former Graduate Students and Postdocs Q12 (Have you spent time working in a laboratory/research group of another CCI partner organization (e.g., another university or company involved with your center) as an intern, graduate student, visiting scholar, or similar role?)

Exhibit I-9a: Type of Partner

	Center for Aerosol Impacts on Climate and the Environ-ment	Center for Chemical Evolution	Center for Chemical Innovation in Solar Fuels	Center for Enabling New Tech-nologies through Catalysis	Center for Selective C-H Functional-ization	Center for Sustainable Materials Chemistry	Center for Sustainable Nano-technology	Center for Sustainable Polymers	Center for Chemistry at the Space-Time Limit	Over-all
Academic institution	100%	100%	100%	79%	85%	100%	82%	100%	100%	91%
Government laboratory	19%	0%	0%	0%	0%	12%	36%	0%	0%	12%
Industry	0%	0%	0%	0%	31%	0%	7%	0%	0%	9%
Foundation/ non-profit	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Other, please specify	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%

Note: Center for Aerosol Impacts on Climate and the Environment (N = 10, missing = 0); Center for Chemical Evolution (N = 4, missing = 0); Center for Chemical Innovation in Solar Fuels (N = 7, missing = 0); Center for Enabling New Technologies through Catalysis (N = 5, missing = 0); Center for Selective C-H Functionalization (N = 13, missing = 0); Center for Sustainable Materials Chemistry (N = 9, missing = 0); Center for Sustainable Nanotechnology (N = 28, missing = 0); Center for Sustainable Polymers (N = 5, missing = 0); Center for Chemistry at the Space-Time Limit (N = 2, missing = 0); Overall (N = 83, missing = 0).

Limited to students who have spent time working in a laboratory/research group of another CCI partner organization.

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Current and Former Graduate Students and Postdocs Q12A (Which of the following best describes the partner organization(s) in which you worked and/or currently work?)

Exhibit I-9b: Time Spent at CCI Partner Organizations

	Percent
3 or fewer months	70%
4 to 6 months	11%
7 to 11 months	3%
12 to 23 months	4%
24 or more months	11%

Note: N = 83, missing = 4

Limited to students who have spent time working in a laboratory/research group of another CCI partner organization.

Source: Survey of Current and Former Graduate Students and Postdocs Q12B_MONTHS (Number of months: How much time did you work at CCI partner organization(s) in total?)

Exhibit I-9c: Value to Career Development

	Center for Aerosol Impacts on Climate and the Environment	Center for Chemical Evolution	Center for Chemical Innovation in Solar Fuels	Center for Enabling New Technologies through Catalysis	Center for Selective C-H Functional-ization	Center for Sustainable Materials Chemistry	Center for Sustainable Nano-technology	Center for Sustainable Polymers	Center for Chemistry at the Space-Time Limit	Over-all
Not at all valuable	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Somewhat valuable	0%	48%	13%	0%	23%	0%	36%	39%	50%	22%
Too early to tell/ uncertain	9%	0%	0%	0%	8%	12%	0%	0%	0%	4%
Very valuable	91%	52%	87%	100%	69%	88%	64%	61%	50%	74%

Note: Center for Aerosol Impacts on Climate and the Environment (N = 10, missing = 0); Center for Chemical Evolution (N = 4, missing = 0); Center for Chemical Innovation in Solar Fuels (N = 7, missing = 0); Center for Enabling New Technologies through Catalysis (N = 5, missing = 1); Center for Selective C-H Functionalization (N = 13, missing = 0); Center for Sustainable Materials Chemistry (N = 9, missing = 0); Center for Sustainable Nanotechnology (N = 28, missing = 0); Center for Sustainable Polymers (N = 5, missing = 0); Center for Chemistry at the Space-Time Limit (N = 2, missing = 0); Overall (N = 83, missing = 1);

Limited to students who have spent time working in a laboratory/research group of another CCI partner organization.

Source: Survey of Current and Former Graduate Students and Postdocs Q12C (How valuable was this experience to your career development?)

Exhibit I-10: Professional Development Opportunities Offered through CCI

	Percent
Research opportunities	88%
Giving presentations	84%
Attending conferences	78%
Publishing papers	78%
Collaborating with researchers outside of your institution	76%
Mentorship	71%
Outreach to the general public	65%
Collaborating with researchers at your institution	62%
Supervising students	49%
Applying for grants/fellowships/awards	40%
Internships/visits to other research labs	33%
Teaching and/or course development	17%
Entrepreneurship	13%

Note: N = 340, missing = 0

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Current and Former Graduate Students and Postdocs Q13 (Which of the following professional development opportunities offered through your CCI have you experienced?)

Exhibit I-11: Satisfaction with these Opportunities

	n	Very Dissatisfied	Dissatisfied	Neutral	Satisfied	Very Satisfied
Research opportunities	300	3%	1%	7%	29%	61%
Giving presentations	288	2%	1%	7%	33%	58%
Attending conferences	270	2%	1%	7%	29%	60%
Publishing papers	269	4%	2%	9%	36%	49%
Collaborating with researchers outside of your institution	263	3%	2%	7%	33%	55%
Mentorship	244	3%	0%	5%	38%	54%
Outreach to the general public	222	1%	0%	10%	38%	51%
Collaborating with researchers at your institution	214	2%	1%	7%	34%	56%
Supervising students	173	1%	0%	7%	38%	54%
Applying for grants/fellowships/awards	139	0%	3%	17%	46%	34%
Internships/visits to other research labs	116	1%	0%	14%	31%	54%
Teaching and/or course development	52	0%	0%	25%	32%	44%
Entrepreneurship	49	0%	4%	13%	43%	40%

Note: N = 50-300, missing = 0-3

Each row limited to respondents who indicated the professional development opportunity was offered through their CCI, according to Q13.

Source: Survey of Current and Former Graduate Students and Postdocs Q14 (How satisfied are you with these opportunities?)

Exhibit I-12: Rating of Experience in CCI

	Percent
Very satisfied	57%
Satisfied	34%
Neutral	6%
Dissatisfied	3%
Very dissatisfied	1%

Note: N = 340, missing = 1

Source: Survey of Current and Former Graduate Students and Postdocs Q15 (Overall, how would you rate your experience in the CCI?)

Exhibit I-13: Advantages and Disadvantages of Participation in CCI

	n	An Advantage	A Disadvantage	No Difference	NA/Too Early to Tell
Breadth of research experience	338	92%	1%	5%	2%
Opportunities to network	337	88%	0%	11%	1%
Access to community of peers	338	87%	2%	10%	2%
Learning about scientific or engineering areas outside of your field	337	81%	1%	17%	1%
Learning how to communicate about your research	338	81%	0%	18%	1%
Ability to advance your research project	337	80%	2%	16%	2%
Access to faculty	338	76%	2%	20%	2%
Access to equipment, facilities, materials, reagents	338	75%	0%	22%	4%
Opportunities to take on leadership responsibilities	337	67%	2%	29%	3%
Quality of training	338	65%	2%	31%	2%
Quality of mentoring	338	65%	3%	30%	2%
Quality of education	338	64%	1%	32%	3%
Ability to develop/work on your own ideas	338	62%	8%	29%	1%
Determining your career direction and options	338	61%	1%	33%	4%
Job opportunities available to you	337	48%	3%	40%	9%
Learning about commercialization and entrepreneurship	337	40%	3%	49%	8%

Note: N = 340, missing = 2-3

Source: Survey of Current and Former Graduate Students and Postdocs Q16 (Please indicate, for each item below, whether participation in CCI has proved to be an advantage, disadvantage, or made no difference)

Exhibit I-14: Participation in CCI

	n	N/A/Too Early to Tell	Well Prepared	Somewhat Prepared	Not Prepared
Current					
Conducting high-quality research	99	2%	87%	10%	1%
Communicating with researchers in your field	100	2%	84%	13%	1%
Working in a multidisciplinary team	100	0%	81%	17%	1%
Presenting and publishing your work	100	1%	76%	22%	2%
Formulating research problems	100	3%	73%	22%	2%
Solving problems which arise in implementing a research program	100	6%	68%	24%	3%
Critically evaluating published literature	100	8%	65%	27%	1%
Communicating with researchers outside of your field	100	5%	58%	32%	6%
Serving as a mentor	99	9%	57%	28%	6%
Communicating research findings to the general public	100	5%	48%	45%	3%
Writing fellowship/grant proposals	99	6%	29%	41%	24%
Working outside of academia	100	10%	27%	43%	20%
Teaching	99	17%	23%	38%	23%
Former					
Conducting high-quality research	237	3%	76%	18%	2%
Communicating with researchers in your field	237	3%	74%	21%	2%
Working in a multidisciplinary team	236	3%	74%	19%	3%
Presenting and publishing your work	237	5%	71%	22%	2%
Critically evaluating published literature	237	4%	62%	29%	5%
Solving problems which arise in implementing a research program	237	6%	60%	27%	6%
Formulating research problems	236	5%	55%	38%	2%
Communicating with researchers outside of your field	237	7%	50%	38%	5%
Serving as a mentor	237	9%	47%	34%	10%
Communicating research findings to the general public	237	6%	45%	39%	10%
Writing fellowship/grant proposals	237	11%	25%	40%	24%
Working outside of academia	236	13%	24%	34%	29%
Teaching	234	15%	20%	42%	23%
Overall					
Conducting high-quality research	336	3%	79%	16%	2%
Communicating with researchers in your field	337	3%	77%	18%	2%
Working in a multidisciplinary team	336	2%	76%	19%	2%
Presenting and publishing your work	337	4%	72%	22%	2%
Critically evaluating published literature	337	6%	63%	28%	4%
Solving problems which arise in implementing a research program	337	6%	62%	26%	5%
Formulating research problems	336	4%	61%	33%	2%
Communicating with researchers outside of your field	337	6%	52%	36%	5%
Serving as a mentor	336	9%	50%	33%	9%

	n	N/A/Too Early to Tell	Well Prepared	Somewhat Prepared	Not Prepared
Communicating research findings to the general public	337	6%	46%	41%	8%
Writing fellowship/grant proposals	336	10%	26%	40%	24%
Working outside of academia	336	12%	25%	37%	26%
Teaching	333	16%	21%	40%	23%

Note: Current (N = 100, missing = 0-1); Former (N = 240, missing = 3-6); Overall (N = 340, missing = 3-7)

Source: Survey of Current and Former Graduate Students and Postdocs Q17 (How well do you think participation in the CCI is preparing you for the following activities?)

Exhibit I-15: Gender

	Percent
Male	62%
Female	35%
Prefer not to report	3%

Note: N = 340, missing = 2

Source: Survey of Current and Former Graduate Students and Postdocs Q18 (What is your gender?)

Exhibit I-16: Underrepresented Ethnic/Racial Minority

	Percent
Yes	12%
No	80%
Prefer not to report	8%

Note: N = 340, missing = 3

Source: Survey of Current and Former Graduate Students and Postdocs Q19 (Do you identify as an underrepresented ethnic/racial minority?)

Exhibit I-16a: Ethnicity

	Percent
Hispanic/Latino	48%
Black or African American	35%
Prefer not to report	13%
Native American	3%
Alaska Native	0%
Native Pacific Islander	0%

Note: N = 42, missing = 0

Limited to respondents who identify as an underrepresented ethnic/racial minority.

Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Current and Former Graduate Students and Postdocs Q19A (Do you identify as an underrepresented ethnic/racial minority? If so, indicate)

Appendix J: Supplemental Tables for Exhibits

This section includes supplemental tables corresponding to the charts included Chapters 3–7.[66] The supplemental tables present percentages measured on the same categorical scale as the corresponding report exhibit, with some categories combined or potentially removed to focus on particular findings (e.g., Satisfied and Very Satisfied combined, Not Applicable removed from denominator). Percentages for survey item response options may differ between the Appendix H and I exhibits and the Appendix J exhibits because the study team excluded respondents who selected Don't Know or Not Applicable from the denominator in the Appendix J exhibits only to match the report exhibits. For ease of finding the corresponding report exhibit, Appendix J exhibits appear in the same order and use the same numbering as those in Chapters 3–7.

[66] A corresponding table for Exhibit 34 was not feasible to prepare, so it is not included in this appendix.

Exhibit J-7: Phase II Investigators Exceeded Pre-award Trends in Publications during Phase I and Maintained High Productivity Levels in Phase II

Publications	Comparison		Phase I-only		Phase I/II	
Year	Average	Linear Prediction	Average	Linear Prediction	Average	Linear Prediction
Years prior to award						
-5	7.03	6.80	6.80	7.18	7.73	7.35
-4	7.05	7.13	7.67	7.78	7.37	7.70
-3	7.09	7.46	8.39	8.38	8.50	8.04
-2	7.66	7.79	8.88	8.98	9.11	8.39
-1	8.16	8.12	9.22	9.58	9.14	8.73
0	8.60	8.45	9.95	10.18	9.06	9.08
Phase I						
1	8.67	8.63	10.01	10.20	10.55	10.28
2	8.75	8.74	10.77	10.99	11.01	11.21
3	8.86	8.85	11.55	11.78	12.43	12.15
Phase II						
4	8.54	8.52	11.68	12.10	11.38	11.29
5	8.28	8.32	11.86	11.39	11.88	11.45
6	8.14	8.12	10.28	10.69	11.63	11.60

Notes: estimated models are interrupted time series, so discontinuities occur at each period boundary. Prediction models include random slopes and intercepts at the individual level and a first-order autoregressive structure.

Source: all publications in Scopus authored by CCI investigators who participated in Phase I. Investigators in the top one percentile of publications are excluded.

Exhibit J-8: CCI Investigators Are More Highly Cited than Comparison Investigators

Citations	Comparison		Phase I-only		Phase I/II	
Year	Average	Linear Prediction	Average	Linear Prediction	Average	Linear Prediction
Years prior to award						
-5	454	429	519	535	533	549
-4	413	427	525	543	521	560
-3	403	424	600	551	566	571
-2	413	421	650	559	523	582
-1	416	419	562	567	619	593
0	433	416	547	575	561	604
Phase I						
1	416	403	651	625	624	644
2	343	367	536	562	561	600
3	342	331	526	499	536	556
Phase II						
4	308	311	441	444	460	502
5	266	259	406	358	490	479
6	203	206	268	272	414	457

Notes: estimated models are interrupted time series, so discontinuities occur at each period boundary. Prediction models include random slopes and intercepts at the individual level and a first-order autoregressive structure.

Source: all publications in Scopus authored by CCI investigators who participated in Phase I. Investigators in the top one percentile of publications are excluded.

Exhibit J-9: Phase II Award Increased Publication Productivity as Measured by CCI-acknowledging Papers

Publications Acknowledging CCI Support	Comparison		Phase I-only		Phase I/II	
Year	Average	Linear Prediction	Average	Linear Prediction	Average	Linear Prediction
Phase I						
0	N/A	N/A	0.00	0.16	0.11	0.07
1	N/A	N/A	2.50	2.04	2.33	2.59
2	N/A	N/A	4.14	3.91	4.33	5.11
3	N/A	N/A	5.64	5.79	7.33	7.62
Phase II						
4	N/A	N/A	4.07	4.16	11.67	12.36
5	N/A	N/A	2.50	2.49	22.78	19.11
6	N/A	N/A	0.79	0.82	25.11	25.86

Notes: estimated models are interrupted time series, so discontinuities occur at each period boundary. Prediction models include random slopes and intercepts at the individual level and a first-order autoregressive structure.
Source: CCI-acknowledging dataset.

Exhibit J-10: CCI-Acknowledging Publications Had Higher Impact Factors than Typical for the Field and Phase I/II Outperformed Phase I-Only Centers

Journal Impact Factor	Comparison (n=2123)	Phase I-only (n=283)	Phase I/II (n=1771)
0 to 0.999	2.1%	0.0%	0.1%
1 to 1.999	9.4%	6.4%	4.6%
2 to 2.999	20.3%	22.3%	11.5%
3 to 3.999	14.6%	9.2%	9.4%
4 to 4.999	14.8%	13.1%	16.4%
5 to 5.999	5.1%	9.2%	5.3%
6 to 6.999	7.1%	5.3%	5.9%
7 to 7.999	1.8%	2.5%	4.1%
8 to 8.999	1.1%	2.1%	1.6%
9 to 9.999	3.5%	2.8%	4.7%
10 to 10.999	1.3%	1.1%	3.2%
11 to 11.999	0.8%	1.1%	0.9%
12 to 12.999	2.5%	5.3%	8.1%
13 to 13.999	0.6%	2.1%	1.5%
14 to 14.999	6.0%	7.1%	12.9%
15 to 19.999	0.5%	0.4%	0.3%
20+	2.8%	6.7%	6.4%
Missing	5.8%	3.5%	3.3%
Mean (Standard Deviation)	6.1 (6.6)	7.9 (8.6)	9.1 (8.8)

Source: CCI-acknowledging dataset and sample of comparison publications. Journal impact factors were obtained from JCR 2018 dataset.

Exhibit J-11: CCI PIs and Co-Investigators Reported Increased Productivity, Diversity of Publications, and Journal Quality

	Increased Due to CCI Participation
Number of papers published per year	65%
Journal quality	43%
Range of journals	45%

Note: N = 134, missing = 5-8

Source: Survey of Principal Investigators and Co-Investigators Q9 (Have any of the following changes occurred in your publication patterns, research interests, and/or professional visibility since you began participating in CCI?)

Exhibit J-12: CCIs Show Leadership by Focusing on Major Scientific Challenges which Require Large Investment of Funds and have the Potential to Radically Advance the Field

	To a Considerable Extent
Focuses on major scientific challenge(s) in fundamental chemistry	97%
Requires a coordinated effort from diverse experts	90%
Has the potential to radically change our understanding of an important scientific or engineering concept	88%
Interdisciplinary	83%
Requires large investment of funds	82%
High-risk	67%
Addresses important societal problem	65%

Note: N = 134, missing = 0-1

Source: Survey of Principal Investigators and Co-Investigators Q4 (To what extent does the research conducted by your CCI have the following characteristics?)

Exhibit J-13: CCI PIs and Co-Investigators Reported Improved Professional Outcomes

	Increased Due to CCI Participation
Number of speaking invitations	47%
Requests to serve as a peer reviewer	43%
Requests to serve on advisory panels	31%
Receipt of awards, fellowships, or chaired positions	28%
Requests to serve on dissertation committees outside your home institution	15%
Requests to serve on editorial board of journals	12%
Requests to provide policy advice or testimony	9%

Note: N = 134, missing = 5-8

Source: Survey of Principal Investigators and Co-Investigators Q9 (Have any of the following changes occurred in your publication patterns, research interests, and/or professional visibility since you began participating in CCI?)

Exhibit J-14: CCI Helped Investigators Generate New Ideas and Broaden Their Research Program

	No Benefit Due to CCI	Some Benefit Due to CCI	Large Benefit Due to CCI
Ideas			
Ability to generate new and/or better ideas	4%	19%	77%
Ability to take your research in a new direction	4%	14%	82%
Ability to more quickly/effectively respond to scientific developments	7%	35%	58%
Resources			
Ability to attract better qualified or more diverse students and postdocs to your research group	7%	34%	58%
Access to resources at partner institutions	8%	41%	51%
Ability to obtain additional funding to support your research	15%	45%	40%
Access to resources at your institution	31%	36%	33%
Tools			
Use of new/additional theoretical or experimental models	8%	32%	59%
Use of new/additional instrumentation or technology	8%	38%	54%
Use of new theoretical models	13%	44%	43%
Use of new/additional data sources	13%	40%	47%

Note: N = 134, missing = 0-1, not applicable = 4-14

Source: Survey of Principal Investigators and Co-Investigators Q8 (Please indicate whether participation in the CCI has benefited your research program.)

Exhibit J-15: Various Resources Created by CCIs are Being Used by Researchers Outside of the Center

	Created by CCI	Used by Unaffiliated Researchers
Methods	83%	73%
Educational or outreach materials	79%	70%
Lessons learned for how to run a large center	77%	45%
New partnerships	75%	43%
Communication infrastructure	57%	26%
Data	57%	60%
Equipment	51%	66%
Facilities	43%	69%
Data management system	39%	27%
Reagents	36%	61%

Note: Q10 N = 134, missing = 0. Q10A N = 111, missing = 0.

Source: Survey of Principal Investigators and Co-Investigators Q10 (Which of the following resources have been created or improved by CCI?); Q10A (Which of these resources, if any, are being used by researchers not affiliated with the center?)

Responses for Q10 may not sum to 100% because multiple responses were permitted. Responses for Q10A are limited to respondents who indicated the resource was created or improved by CCI in Q10.

Exhibit J-18: Benefits of CCI to Industry Include Ideas, Staff, Products, and Reduction in Environmental Impact

	Some Benefit Due to CCI	Large Benefit Due to CCI
New or improved ideas for commercial product or process	40%	32%
Access to personnel	28%	42%
New or improved product or process	38%	28%
Reduction in environmental impact	30%	21%
Ability to meet regulatory requirements	17%	3%
Cost savings	11%	3%
Increase in sales	6%	1%

Note: N = 134, missing = 5-12

Source: Survey of Principal Investigators and Co-Investigators Q14 (Please indicate whether the CCI delivered any of the following benefits to industry.)

Exhibit J-19: More than Half of Graduate Students and Postdocs Had Multiple Mentors

	Graduate Student	Postdoc
Single mentor who participates in CCI	38%	49%
Multiple mentors who all participate in CCI	35%	41%
Multiple mentors, but not all of them participate in CCI	23%	10%

Note: Graduate Student (N = 227, missing = 0); Postdoc (N = 113, missing = 0); Overall (N = 340, missing = 0).

Source: Survey of Current and Former Graduate Students and Postdocs Q7 (How many people served as mentors to you (either formally or informally), providing guidance, feedback, and support for your development and research?)

Exhibit J-20: Graduate Students and Postdocs Were Satisfied with a Broad Range of Career Development Opportunities Available at CCIs

	Experienced	Satisfied or Very Satisfied
Research opportunities	88%	89%
Giving presentations	84%	91%
Attending conferences	78%	90%
Publishing papers	78%	85%
Collaborating with researchers outside of your institution	76%	88%
Mentorship	71%	92%
Outreach to the general public	65%	89%
Collaborating with researchers at your institution	62%	90%
Supervising students	49%	92%
Applying for grants/fellowships/awards	40%	80%
Internships/visits to other research labs	33%	85%
Teaching and/or course development	17%	75%
Entrepreneurship	13%	83%

Note: Q13 Note: N = 340, missing = 0; Q14 N = 50-300, missing = 0-3.

Source: Survey of Current and Former Graduate Students and Postdocs Q13 (Which of the following professional development opportunities offered through your CCI have you experienced?), Q14 (How satisfied are you with these opportunities?)

Responses for Q13 may not sum to 100% because multiple responses were permitted. Responses for Q14 are limited to respondents who indicated the professional development opportunity was offered through their CCI in Q13.

Exhibit J-21: Most Graduate Students and Postdocs Who Worked at a Partner Organization Found the Experience Very Valuable

	Worked at Partner	Found Experience Very Valuable
CSN – Center for Sustainable Nanotechnology	57%	64%
CAICE – Center for Aerosol Impacts on Climate and the Environment	31%	91%
CCHF – Center for Selective C-H Functionalization	27%	69%
Solar – Center for Chemical Innovation in Solar Fuels	24%	87%
CSMC – Center for Sustainable Materials Chemistry	21%	88%
CCE – Center for Chemical Evolution	17%	52%
CSP – Center for Sustainable Polymers	12%	61%
CENTC – Center for Enabling New Technologies through Catalysis	9%	100%
CaSTL – Center for Chemistry at the Space-Time Limit	8%	50%

Note: CAICE (N = 10, missing = 0); CCE (N = 4, missing = 0); Solar (N = 7, missing = 0); CENTC (N = 5, missing = 1); CCHF (N = 13, missing = 0); CSMC (N = 9, missing = 0); CSN (N = 28, missing = 0); CSP (N = 5, missing = 0); CaSTL (N = 2, missing = 0); Overall (N = 83, missing = 1).

Source: Survey of Current and Former Graduate Students and Postdocs Q12 (Have you spent time working in a laboratory/research group of another CCI partner organization (e.g., another university or company involved with your center) as an intern, graduate student, visiting scholar, or similar role?); Q12C (How valuable was this experience to your career development?)

Exhibit J-22: Professional Development Opportunities Available at CCIs Were an Advantage

	A Disadvantage	No Difference	An Advantage
Breadth of research experience	1%	5%	94%
Opportunities to network	0%	11%	89%
Access to community of peers	2%	10%	88%
Learning about scientific or engineering areas outside of your field	1%	17%	82%
Ability to advance your research project	2%	16%	82%
Learning how to communicate about your research	0%	18%	82%
Access to faculty	2%	20%	78%
Access to equipment, facilities, materials, reagents	0%	22%	78%
Opportunities to take on leadership responsibilities	2%	30%	69%
Determining your career direction and options	2%	35%	64%
Ability to develop/work on your own ideas	8%	29%	63%
Job opportunities available to you	3%	44%	53%
Learning about commercialization and entrepreneurship	3%	54%	44%

Note: N = 340, missing = 2-3, Not applicable/too early to tell =2-33.

Source: Survey of Current and Former Graduate Students and Postdocs Q16 (Please indicate, for each item below, whether participation in CCI has proved to be an advantage, disadvantage, or made no difference)

Exhibit J-23: CCI Prepared Graduate Students and Postdocs for Research Careers

	Not Prepared	Somewhat Prepared	Well Prepared
Conducting high-quality research	2%	16%	82%
Presenting and publishing your work	2%	23%	75%
Communicating with researchers in your field	2%	19%	79%
Formulating research problems	2%	34%	63%
Working in a multidisciplinary team	2%	19%	78%
Critically evaluating published literature	4%	30%	66%
Solving problems which arise in implementing a research program	6%	28%	66%
Communicating with researchers outside of your field	6%	39%	56%
Communicating research findings to the general public	8%	43%	49%
Serving as a mentor	10%	36%	55%
Writing fellowship/grant proposals	27%	44%	29%
Teaching	27%	48%	25%
Working outside of academia	30%	42%	28%

Note: N = 340, missing = 3-7, Not applicable/too early to tell=8-52.

Source: Survey of Current and Former Graduate Students and Postdocs Q17 (How well do you think participation in the CCI is preparing you for the following activities?)

Exhibit J-24: CCI Prompted Some Graduate Students and Postdocs to Change Their Career Goals

	Grad Student		Postdoc	
	Goal Before CCI	Goal Since CCI	Goal Before CCI	Goal Since CCI
Research and development position in industry	56%	33%	48%	22%
Faculty member in a research college or university	57%	10%	80%	17%
Researcher in a government laboratory	34%	31%	46%	19%
Faculty member in a 2-year or 4-year teaching college	41%	11%	38%	8%
Science policy, law, consulting, or science writing	18%	28%	21%	0%
Non-tenure-track researcher in a university or a research institute	15%	21%	13%	5%
Business position in industry or an entrepreneur	25%	10%	15%	13%
Program officer/academic administrator	7%	7%	15%	11%

Note: Graduate Student (N = 82, missing = 0-6); Postdoc (N = 18, missing = 0-2). Limited to current students.

Source: Survey of Current and Former Graduate Students and Postdocs Q11 (Which of the following positions are you most interested in pursuing after you complete your degree and/or postdoctoral training? Have your career goals changed since you began participating in the CCI?)

Exhibit J-25: For Many Students and Postdocs, CCI Influenced the Choice of Institution, Problem, Field of Study, and Advisor

	Graduate Student	Postdoc
Type of institution to join	43%	39%
Whether to pursue postdoctoral training	42%	9%
Choice of research problem	37%	50%
Choice of discipline/field of study	33%	36%
Choice of advisor/mentor	25%	16%
Choice of specific employer	13%	10%

Note: Graduate Student (N = 145, missing = 0); Postdoc (N = 95, missing = 0)

Source: Survey of Current and Former Graduate Students and Postdocs Q8 (Did your CCI experiences influence any of these choices?) Responses may not sum to 100% because multiple responses were permitted. Responses were limited to past students.

Exhibit J-26: Most Former Graduate Students and Postdocs are Employed in Academia or Industry

	Graduate Student	Postdoc
College or university	32%	60%
Industry (chemical or pharmaceutical company or similar)	36%	20%
Government (including government research labs)	14%	9%
Research institution/think tank	3%	4%
Non-government lab	1%	3%
Entrepreneur/self-employed	2%	1%
Other nonprofit organization or private foundation	2%	0%
Other	7%	3%
Not employed	4%	0%

Note: Graduate (N = 126, missing = 0); Postdoc (N = 94, missing = 0)

Source: Survey of Current and Former Graduate Students and Postdocs Q10 (Which of the following best describes your current principal employer?) Responses were limited to past students not currently enrolled in a degree program.

Exhibit J-27: CCIs Developed or Improved Mechanisms to Support URGs Which They Viewed as Effective

CCI PIs and Co-Investigators who reported that the center…	
Developed or Improved mechanisms for recruitment and/or retention of individuals from URGs	74%
Developed or Improved mechanisms for mentorship of individuals from URGs	68%
Engagement with organizations with expertise supporting URGs in the scientific community	63%
Increased participation of URGs in their lab	78%
Increased participation of URGs at their institution	64%
Were more successful because of broadening participation activities and programs	98%

Note: Q11 (N = 134, missing = 0); Q13 (N = 134, missing = 4-6); Q16 "Broadening Participation" (N = 123, missing = 11)

Source: Survey of Principal Investigators and Co-Investigators Q11 (Please indicate whether your CCI developed or improved the following educational and/or outreach opportunities.). Q13 (Please indicate whether the following improvements have occurred as a result of CCI funding). Q16 (To what extent have these elements contributed to the success of your center?).

Exhibit J-28: Representation of URGs at CCIs was Similar for Gender and Slightly Better for Racial/Ethnic Diversity than the National Averages

	CCI Participants	2017 Chemistry PhD Recipients
Female	36%	38%
Underrepresented Minority	13%	9%

Note: N = 340, missing = 2

Source: Survey of Current and Former Graduate Students and Postdocs Q18 (What is your gender?); Q19 (Do you identify as an underrepresented ethnic/racial minority?); National Science Foundation, Survey of Earned Doctorates, Doctorate recipients, by sex and major field of study: 2008–17 (Table 15); National Science Foundation, Survey of Earned Doctorates, U.S. citizen and permanent resident doctorate recipients, by major field of study, ethnicity, and race: 2017 (Table 24)

Exhibit J-29: CCIs Established Many Programs to Educate the Public about Chemistry Which They Viewed as Effective

CCI PIs and Co-Investigators who reported that the center…	
Developed or improved programs for educating the public about chemistry	86%
Improved engagement with organizations focused on outreach and advocacy to pre-college, public, or policy-maker audiences	64%
Were more successful because of public outreach activities and programs	96%
Increased interest in/understanding of chemistry among the public	82%

Note: Q11 (N = 134, missing = 0); Q13 (N = 134, missing = 4-6); Q16 "Public Outreach" (N = 122, missing = 12)

Source: Survey of Principal Investigators and Co-Investigators Q11 (Please indicate whether your CCI developed or improved the following educational and/or outreach opportunities.). Q13 (Please indicate whether the following improvements have occurred as a result of CCI funding). Q16 (To what extent have these elements contributed to the success of your center?).

Exhibit J-30: CCI Investigators Believed that Many of Their Programs Will Be Sustained after the End of the Grant

	Developed	Will Sustain
Research and teaching experiences for students and postdocs	88%	70%
Programs for educating the public about chemistry	86%	64%
Mechanisms for recruitment and/or retention of individuals from underrepresented groups	74%	58%
Mechanisms for mentorship of individuals from underrepresented groups	68%	65%
Engagement with organizations focused on outreach and advocacy to pre-college, public, or policymaker audiences	64%	44%
Engagement with organizations with expertise supporting underrepresented groups in the scientific community	63%	61%
Courses/seminars in chemistry	63%	69%
Training programs in chemistry	61%	47%

Note: Q11 N = 134, missing = 0; Q12 N = 117, missing = 0.

Source: Survey of Principal Investigators and Co-Investigators Q11 (Please indicate whether your CCI developed or improved the following educational and/or outreach opportunities.), Q12 (Please indicate whether you expect to be able to sustain the following programs and activities after the grant ends. If your grant has ended, please indicate whether these programs and activities are still in place)

Responses for Q11 may not sum to 100% because multiple responses were permitted. Responses for Q12 are limited to respondents who indicated that the opportunity was developed or improved by their CCI in Q11.

Exhibit J-31: CCI PIs and Co-Investigators were Satisfied with the Partnerships

A. Satisfaction	Satisfied	Very Satisfied
Communication tools	48%	35%
Productivity of meetings among partners	47%	36%
Frequency of meeting among partners	47%	34%
Intellectual contribution of partners	36%	52%
Sharing of credit among partners	38%	44%
Distribution of resources among partners	35%	41%
B. Challenges	**Experienced Challenge**	**Resolved to Some or Considerable Extent**
Terminating unsuccessful projects	42%	94%
Coordination of activities between partners	40%	95%
Communication between partners	38%	93%
Contributions by partners to the center	25%	92%
Sharing of credit for discovery	21%	82%
Access to needed resources	17%	91%

Note A: N = 134, missing = 5-22, N/A = 2-36.

Source A: Survey of Principal Investigators and Co-Investigators Q15 (How satisfied are you with the following elements of CCI?)

Note B: Q18 N = 134, missing = 0; Q19 Note: N = 79, missing = 0-3,

Source B: Survey of Principal Investigators and Co-Investigators Q18 (Has your CCI experienced the following challenges?), Q19 (To what extent have these challenges been resolved?)

Responses for Q18 may not sum to 100% because multiple responses were permitted. Responses for Q19 are limited to respondents who indicated that the challenge had been experienced, according to Q18.

Exhibit J-32: Many Investigators Experienced Technical or Partnership Challenges, but These were Typically Resolved

	Experienced Challenge	Resolved to Some or Considerable Extent
Technical or experimental challenges	58%	98%
Delays in progress of research	33%	95%
Meeting administrative requirements	31%	95%
Staffing of the center	21%	97%
Seeding new projects	18%	97%

Note: Q18 N = 134, missing = 0; Q19 N = 79, missing = 0-3,

Source: Survey of Principal Investigators and Co-Investigators Q18 (Has your CCI experienced the following challenges?), Q19 (To what extent have these challenges been resolved?)

Responses for Q18 may not sum to 100% because multiple responses were permitted. Responses for Q19 are limited to respondents who indicated that the challenge had been experienced, according to Q18.

Exhibit J-33: Researchers Who Received Phase II Awards Continued to Generate Joint Publications While Those Who Did Not Reverted to the Pre-CCI Co-Authorship Level

Percentage of Publications with CCI Co-Authors	Comparison		Phase I-only		Phase I/II	
Year	Average	Linear Prediction	Average	Linear Prediction	Average	Linear Prediction
Years prior to award						
-5	N/A	N/A	6%	7%	7%	6%
-4	N/A	N/A	6%	8%	9%	7%
-3	N/A	N/A	8%	9%	10%	8%
-2	N/A	N/A	10%	11%	9%	9%
-1	N/A	N/A	10%	12%	11%	10%
0	N/A	N/A	12%	13%	14%	11%
Phase I						
1	N/A	N/A	13%	13%	16%	12%
2	N/A	N/A	14%	18%	17%	20%
3	N/A	N/A	23%	23%	30%	27%
Phase II						
4	N/A	N/A	13%	15%	24%	23%
5	N/A	N/A	17%	14%	31%	27%
6	N/A	N/A	11%	14%	31%	31%

Notes: estimated models are interrupted time series, so discontinuities occur at each period boundary. Prediction models include random slopes and intercepts at the individual level and a first-order autoregressive structure.

Source: all publications in Scopus authored by CCI investigators who participated in Phase I. Investigators in the top one percentile of publications are excluded.

Exhibit J-35: The Majority of Participants Are More Satisfied with Communication than Data Sharing Tools Developed by their CCI

	Satisfied	Very Satisfied
Communication tools	48%	35%
Data sharing tools	45%	22%

Note: N = 134, missing = 5-22, N/A = 2-36

Source: Survey of Principal Investigators and Co-Investigators Q15 (How satisfied are you with the following elements of CCI?)

Exhibit J-36: The Majority of Participants Reported that Communication and Data Sharing Tools Contributed to Success of their CCI

	Not at all	Some	Considerable
Communication tools	4%	48%	48%
Data sharing tools	17%	57%	26%

Note: N = 85-127, missing = 6-24. Each row is limited to respondents who were not dissatisfied with the element, according to Q15.

Source: Survey of Principal Investigators and Co-Investigators Q16 (To what extent have these elements contributed to the success of your center?)

Exhibit J-37: CCI Investigators Were More Satisfied with the Funding Level and Duration of Phase II than of Phase I

	Satisfied	Very Satisfied
Funding Level for Phase I	39%	34%
Duration of Phase I	42%	35%
Funding level for Phase II	35%	55%
Duration of Phase II	34%	53%

Note: N = 134, missing = 5-22, N/A = 2-36.

Source: Survey of Principal Investigators and Co-Investigators Q15 (How satisfied are you with the following elements of CCI?)

Exhibit J-38: Funding Level and Duration of Phase II were More Important to the Success of the Center than of Phase

	To Some Extent	To a Considerable Extent
Funding Level for Phase I	46%	50%
Duration of Phase I	49%	46%
Funding level for Phase II	22%	76%
Duration of Phase II	18%	80%

Note: N = 85-127, missing = 6-24. Each row is limited to respondents who were not dissatisfied with the element, according to Q15.

Source: Survey of Principal Investigators and Co-Investigators Q16 (To what extent have these elements contributed to the success of your center?)

Exhibit J-39: The Two-Phase Model Allowed Participants and NSF to Select and Build Better Centers

	Overall
It allows the centers to refine their research goals and approach	83%
It enables selection of better Phase II centers by NSF	69%
It allows the centers to pilot activities and programs	67%
It allows selection of the right partners	65%
It allows the centers to develop and test policies and procedures	51%
It allows participants to determine whether they like the experience	37%
Other advantages	2%
No advantages	6%

Note: N = 134, missing = 4; Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q23 (In your view, which of the following are the advantages of the two-phase model?)

Exhibit J-40: Phase I-Only and Phase I/II Investigators Differ on Their Views of the Two-Phase Model

	Phase I-Only	Phase I/II
It allows the centers to refine their research goals and approach*	58%	86%
It enables selection of better Phase II centers by NSF***	28%	75%
It allows the centers to pilot activities and programs	62%	67%
It allows selection of the right partners	54%	67%
It allows the centers to develop and test policies and procedures*	28%	54%
It allows participants to determine whether they like the experience	19%	40%
Other advantages	0%	2%
No advantages*	17%	5%

** indicates significance level: * ($p < 0.05$), ** ($p < 0.01$), *** ($p < 0.001$).*

Note: Phase I (N = 18, missing = 2), Phase II (N = 116, missing = 2), overall (N = 134, missing = 4); Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q23 (In your view, which of the following are the advantages of the two-phase model?)

Exhibit J-41: Almost All Phase II Investigators and under Half of Phase I Investigators Prefer a Two-Phase Model

	1-Phase Model is Preferable	Uncertain	2-Phase Model is Preferable
Phase I-only investigators	38%	19%	43%
Phase I/II investigators	6%	15%	80%

Note: Phase I (N = 18, missing = 3), Phase II (N = 116, missing=3), overall (N = 134, missing = 6). Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q25 (On balance, is a two-phase center model preferable to a single phase?).

Exhibit J-42: Phase I Helped Investigators Form and Sustain Collaborations, Advance their Research, Train Students, Develop Outreach Programs, and Learn how to Run Centers

	Occurred Due to Phase 1 Participation
Formed new or cemented old collaborations	80%
Advanced your research program	75%
Provided training or career development opportunities for students or postdocs	73%
New direction for your research program	71%
Gained experience of participating in or running a center	67%
Developed educational or public outreach programs	56%
Developed center policies and procedures	46%
Obtained additional funding to support your research	45%
Other benefits	3%
No benefits of participation in Phase I	3%

Note: N = 92, missing = 4. Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q21 (Have any of the following occurred as a result of your participation in Phase I?).

Exhibit J-43: Disadvantages of the Two-Phase Model Include Insufficient Resources to Continue the Research and Time Lost in Submitting an Application for Phase I-Only Centers

	Phase I-Only	Phase I/II
Insufficient resources for Phase I grantees not selected for Phase II to continue their research***	79%	33%
Time burden to submit a Phase II application	51%	35%
Some strong applicants may be discouraged from applying	26%	17%
Other disadvantages	36%	8%
Delay in tacking time-sensitive topics***	<1%	12%
No disadvantages***	0%	5%

** indicates significance level: * (p < 0.05), ** (p < 0.01), *** (p < 0.001)*

Note: Phase I (N = 18, missing = 2), Phase II (N = 116, missing = 2), overall (N = 134, missing = 4). Responses may not sum to 100% because multiple responses were permitted.

Source: Survey of Principal Investigators and Co-Investigators Q24 (In your view, what are the disadvantages of the two-phase model?)

Appendix K: Phase II Chord Diagrams

This appendix contains chord diagrams that illustrate patterns of co-authorship within the nine Phase I/II centers. See Chapter 2 (Methodology) for details on how the diagrams were created. Each colored segment along the perimeter of the chord diagram represents a CCI investigator, and the arcs between two colored segments represent co-authored publications. The width of the arc is proportional to the number of publications co-authored by the two investigators. The variation in size of the perimeter segments demonstrate whether collaboration within a center is largely shouldered by a few key investigators or more evenly spread amongst all investigators. The number of arcs terminating in each perimeter segment illustrates whether an investigator has a broad network of collaborators or exclusively publishes with one or two other investigators in the center.

Exhibit K-1: Center for Enabling New Technologies through Catalysis Chord Diagram

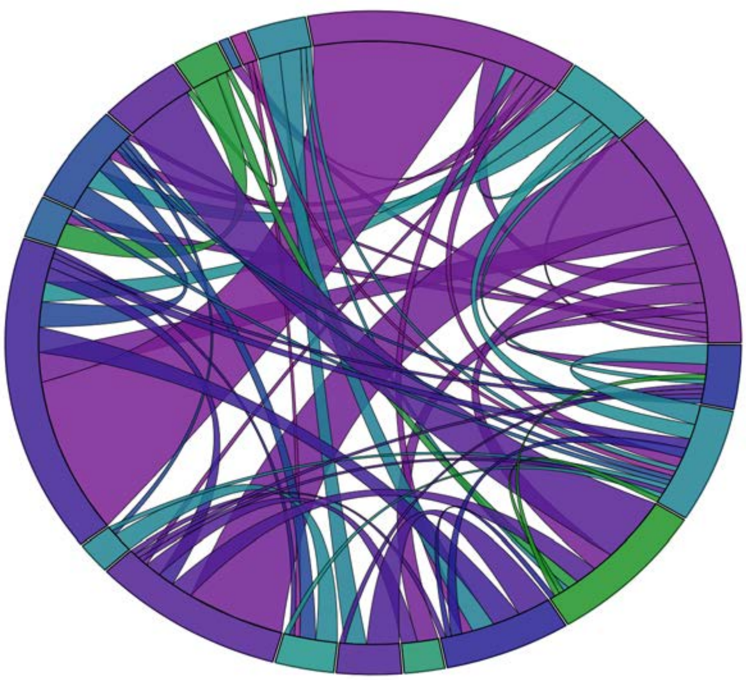


Exhibit K-2: Center for Chemical Innovation in Solar Fuels Chord Diagram

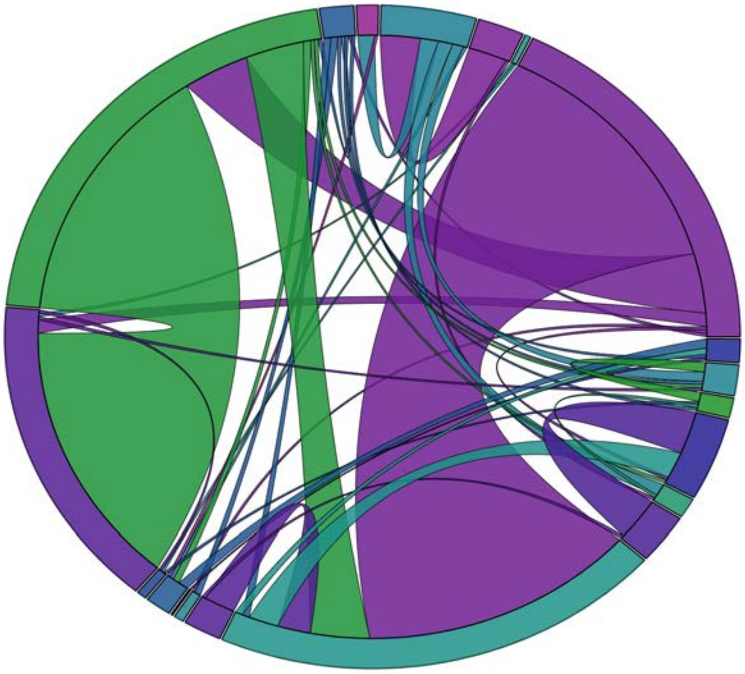


Exhibit K-3: The Center for Chemistry at the Space-Time Limit Chord Diagram

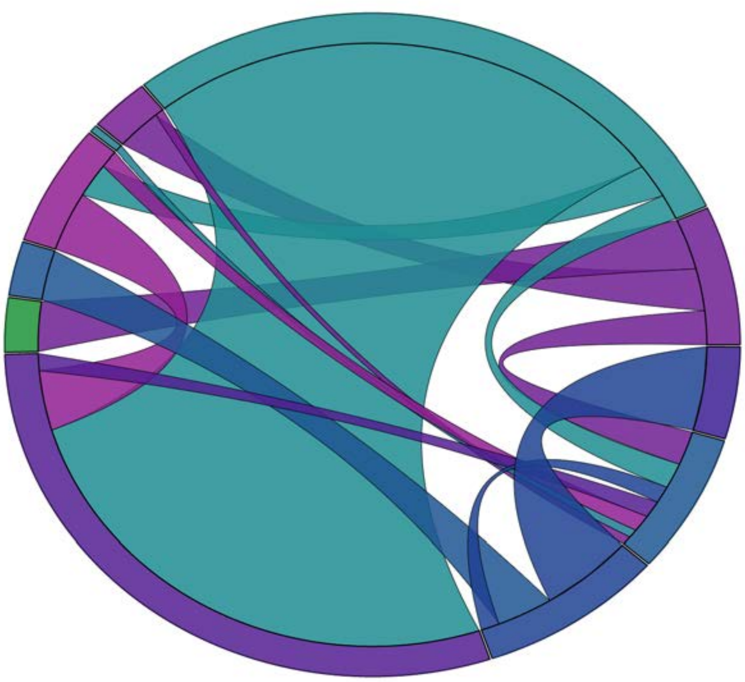


Exhibit K-4: Center for Chemical Evolution Chord Diagram

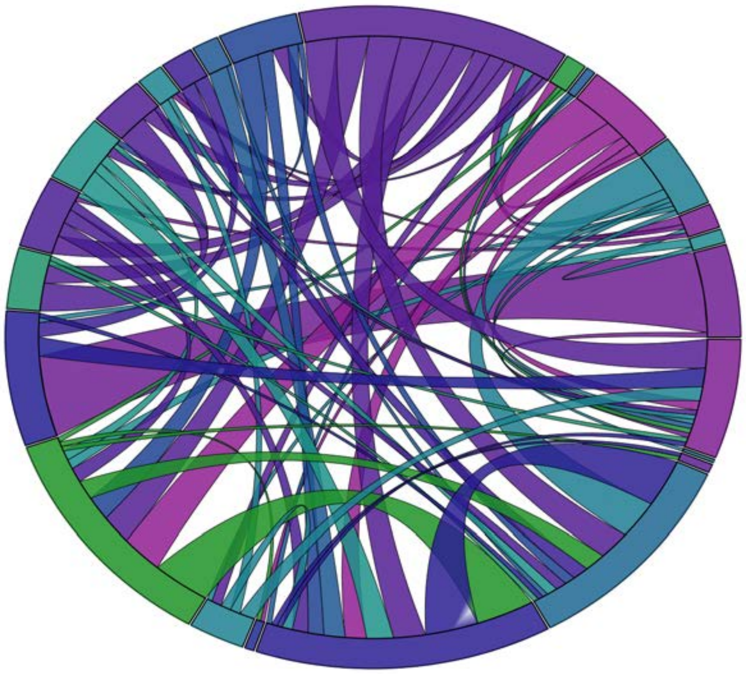


Exhibit K-5: Center for Sustainable Materials Chemistry Chord Diagram

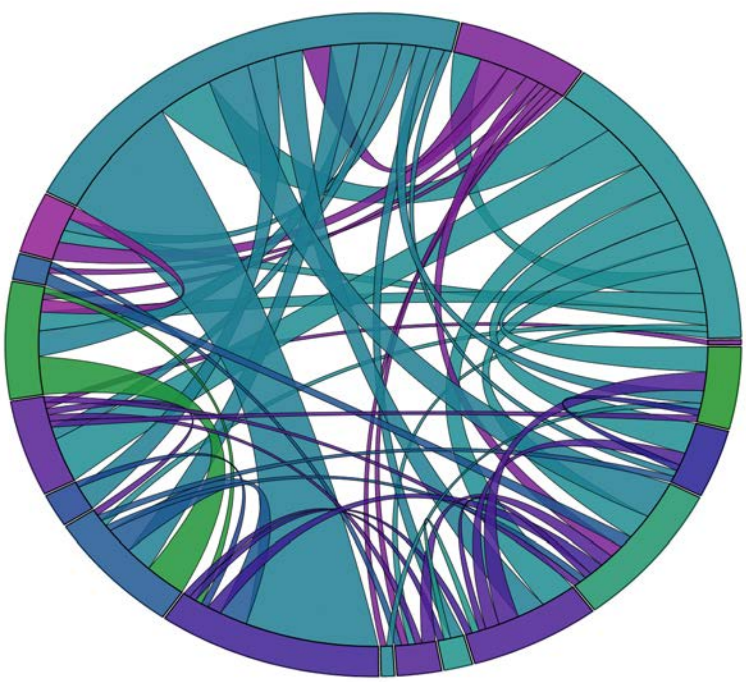


Exhibit K-6: Center for Selective C-H Functionalization Chord Diagram

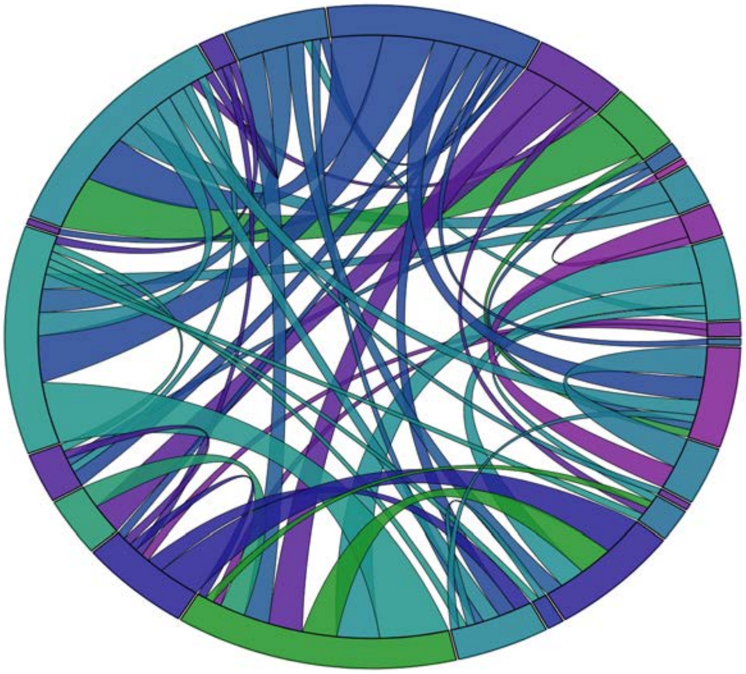


Exhibit K-7: Center for Aerosol Impacts on Climate and the Environment Chord Diagram

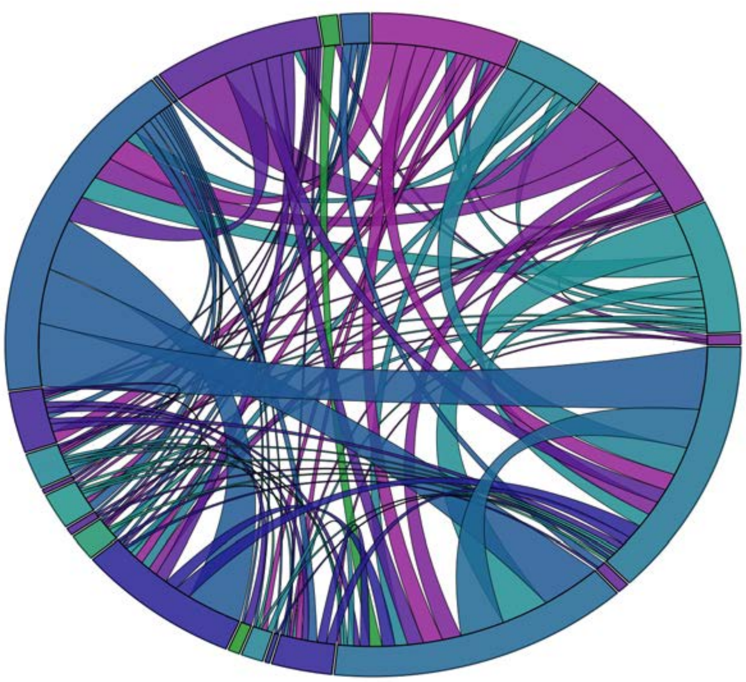


Exhibit K-8: Center for Sustainable Polymers Chord Diagram

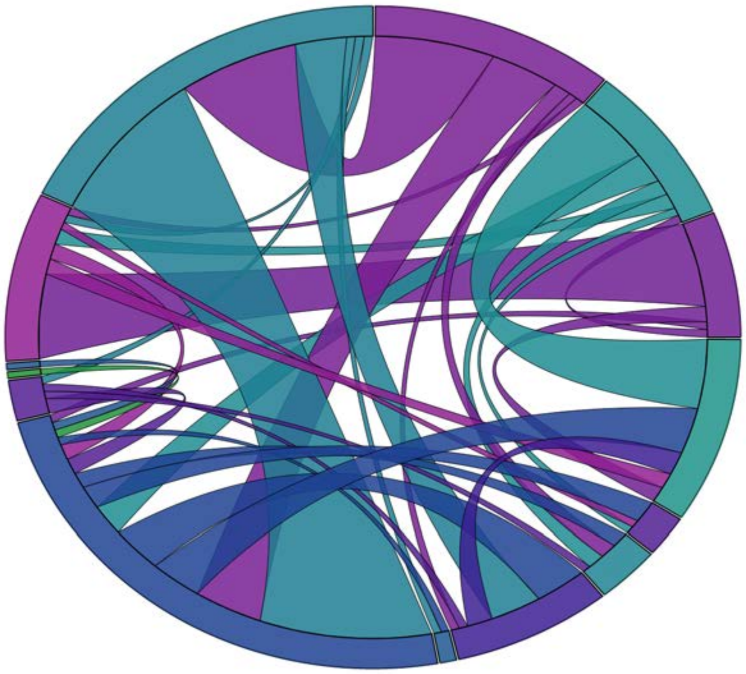


Exhibit K-9: Center for Sustainable Nanotechnology Chord Diagram