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

## EXECUTIVE SUMMARY

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# 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.

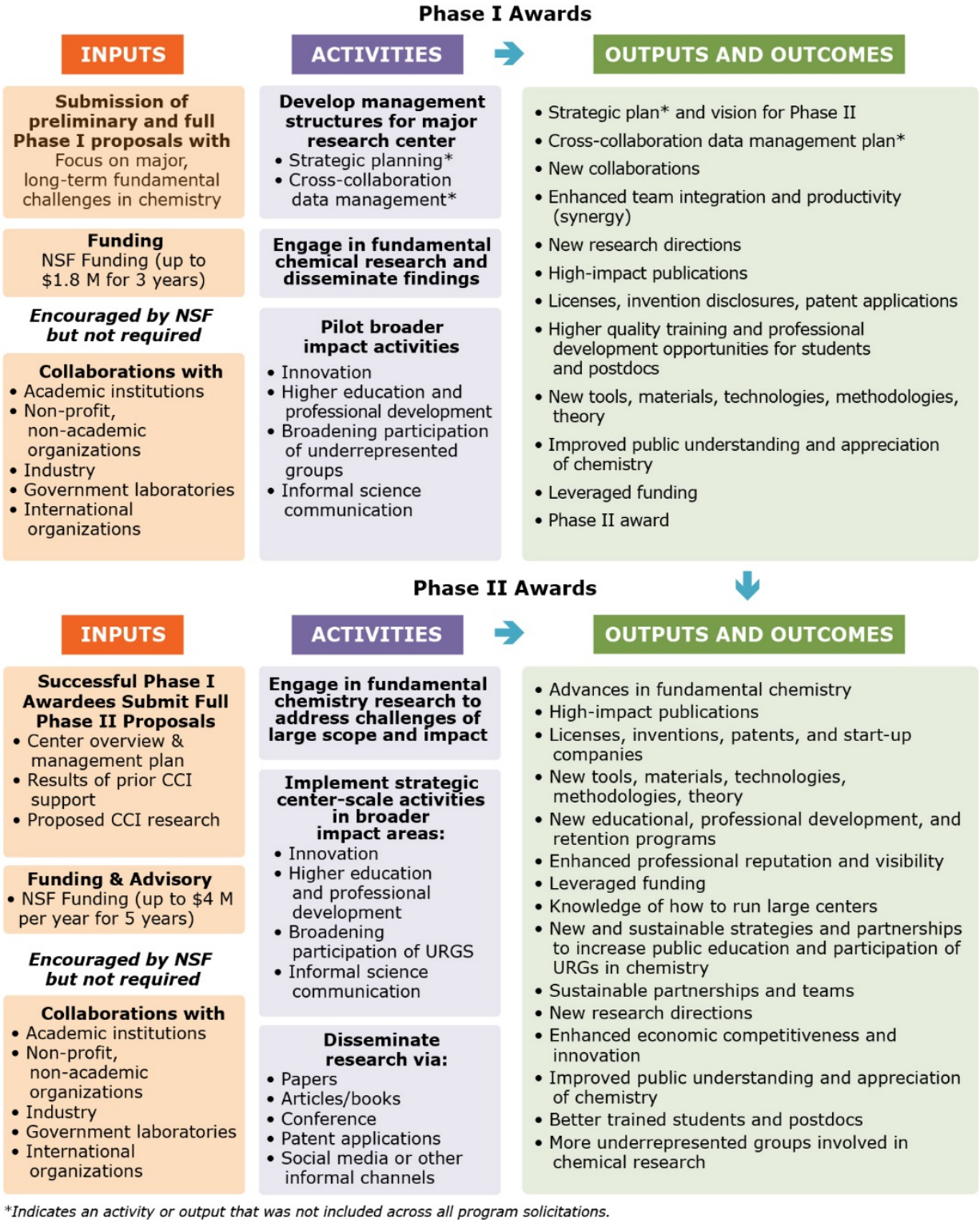
The CCI Program uses a two-phase funding mechanism. In Phase I, grantees receive up to $1.8 million for three years to conduct research; contribute to the broader impact goals of NSF; and develop the infrastructure, vision, programs, and partnerships for a major research center. All grantees are eligible 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**




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

The evaluation addressed five broad research questions:[1]

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|---|---|
| 1 | **What are the important contributions of the CCI Program to our current understanding of fundamental chemistry?**[2,3] |
| 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[4] 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.


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

2 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.

3 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.

4 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.[5] 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.[6] 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),[7] 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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5 This number represents every record associated with these investigators available in Scopus through early 2019, including peer reviewed articles, books, and conference papers.

6 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.

7 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.[8]
- **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.

[8] 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).

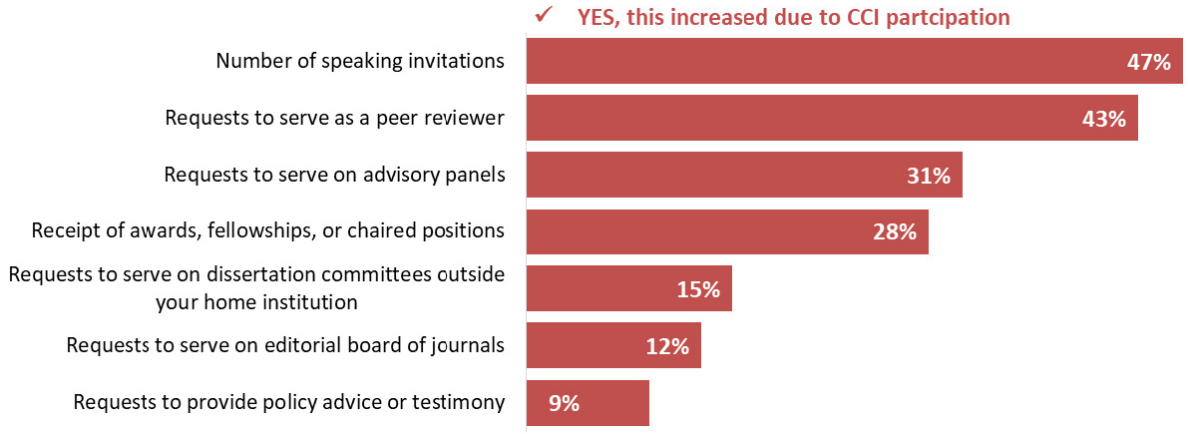
**Benefits to the chemistry research community**

- 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.

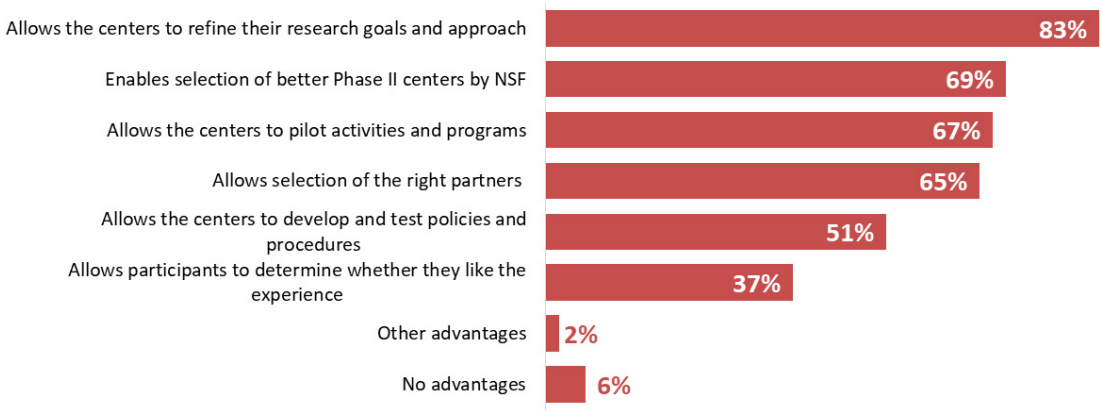
## Research Question 5: How effective is the two-phase funding model for the CCI Program?

- 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.