



## NSF Convergence Accelerator's 2022 Cohort Phase 1 Award

### Project Title

PFASTIR: PFAS Toolkit for Innovating Replacements

### Awardee

IBM Corporation through its Almaden Research Center

### Award/Contract #

49100423C0007

### Award Contract Type

R&D

### Award Date

December 15, 2022

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### NSF Funded Program

NSF's Convergence Accelerator

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### PROJECT ABSTRACT

Per- and polyfluoroalkyl substances (PFAS), a large set of organofluorine compounds and materials, are an important class of persistent environmental pollutants with harmful environmental and human health impacts. The identification, assessment, replacement, and remediation of PFAS chemicals and materials is an urgent global sustainability challenge. Critically, the recent expansion of the PFAS class definition has scaled the problem far beyond what traditional chemical and material discovery paradigms can manage. To create a comprehensive and scalable solution for accelerating the discovery of PFAS replacements, IBM will partner with OntoChem, the University of Pittsburgh, Cornell University, and NuMat Technologies with additional guidance from the Semiconductor Industry Association (SIA) PFAS Consortium and the Division of the National Toxicology Program – National Institute of Environmental Health Sciences (DNTP/NIEHS).

The PFAS Toolkit for Innovating Replacements (PFASTIR) program converges knowledge-centric systems, computational tools, and multiple scientific disciplines to develop data and tools to accelerate the design of environmentally sustainable chemicals, materials, and processes intended to replace, capture, and/or destroy PFAS chemicals and materials. Our vision includes tools such as (a) a PFAS knowledge hub with comprehensive coverage of PFAS chemicals, including classifications, associations with roles and applications, physicochemical properties, etc., (b) predictive models for physicochemical properties, transformations under environmental and industrial conditions, environmental and toxicology endpoints, selective capture by absorbent materials, etc., and (c) a framework for a multi-dimensional level-of-knowledge assessment of PFAS molecules and classes to reveal important knowledge gaps.

PFASTIR will benefit stakeholders who need to quickly understand a specific or general PFAS problem statement, efficiently identify opportunities for discovering more sustainable replacements and/or reduce environmental impact via PFAS capture/remediation, and/or accelerate research efforts to design those PFAS replacement or capture materials.