NATIONAL SCIENCE FOUNDATION
2415 EISENHOWER AVENUE
ALEXANDRIA, VIRGINIA 22314

NSF 20-017

Dear Colleague Letter: Research Opportunities for the Directorate for Mathematical and Physical Sciences (MPS) in Artificial Intelligence Research Institutes

November 7, 2019

Dear Colleagues:

Recent ground-breaking advances in artificial intelligence (AI) have been enabled by increased computing power, algorithmic improvements in machine-learning, and the availability of large data sets. Synergies between research frontiers in AI and Mathematical and Physical Sciences (MPS) have the potential to stimulate further transformative progress in both fields. The National Artificial Intelligence Research Institutes program (described in NSF 20-503) supports teams of scientists, engineers, and educators in multidisciplinary efforts that advance AI and contribute to research challenges in other domains of science and engineering. National AI Research Institutes are characterized by their commitment to pursuing foundational AI research, advancing domain science by leveraging use-inspired AI research, actively building the next generation of talent, and creating a nexus for collaborative

This Dear Colleague Letter (DCL) describes opportunities for MPS researchers to participate in the National AI Research Institutes program. There are two tracks described in the Program Solicitation: a Planning Grant track and an Institute Track that has six specific thematic areas. Two of the Institutes Tracks may be of particular interest to researchers working in the fields of Chemistry (CHE) / Chemical, Bioengineering, Environmental and Transport Systems (CBET) and Physics:

- AI for Accelerating Molecular Synthesis and Manufacturing and
- AI for Discovery in Physics

Please note that a webinar answering questions on the National AI Institutes will be given on Thursday, November 7 from 3:30-4:30 pm (EST). Please register online at https://www.nsf.gov/events/event_summ.jsp?cntn_id=299439&org=CISE.

PROPOSAL DEADLINES:

1. Planning Grant Track: January 30, 2020
2. Institute Track: January 28, 2020

INSTITUTE TRACKS

AI FOR ACCELERATING MOLECULAR SYNTHESIS AND MANUFACTURING

Constant demands for new molecule discovery, alternative, and adaptable chemical synthesis routes, and the development of energy-efficient chemical manufacturing processes are often hampered by labor-intensive and intuition-driven synthetic optimization. The innovative development of AI tools to learn, analyze, and predict multi-dimensional reactivity trends and alternative synthetic pathways has the potential to instigate revolutionary advances in synthetic chemistry addressing these historical roadblocks. The AI for Accelerating Molecular Synthesis and Manufacturing Research Institute Track seeks to support teams who plan to combine pioneering AI designs for multi-source data collection, machine-readable data representation, and learning algorithms that incorporate reaction rules and molecular properties with creative approaches for predictive synthesis and characterization to achieve ground-breaking advances that address the need for enhanced discovery and improved manufacturing in chemistry.

It is anticipated that moderate automated synthetic instrumentation purchases may be requested to facilitate high throughput synthesis as well as in situ and ex situ characterization in the development of safer, more reproducible, and more sustainable molecular synthesis and chemical engineering processes.

This track is currently restricted to molecular chemistry targets (including macromolecular, supramolecular and nanochemistry). Proposers are also reminded that NSF does not support disease-related research; proposals focused on drug discovery and testing toward specific disease targets will be returned without review. Investigators are strongly urged to contact the cognizant Program Officers (see below) if they have questions on target scope.

AI FOR DISCOVERY IN PHYSICS

Investigators are strongly encouraged to contact the cognizant Program Officers (see below) if they have questions on the AI for Discovery in Physics track described in the solicitation.

PLANNING GRANT TRACK

This program provides a funding opportunity for two-year planning grants for groups of researchers to develop communities, capacity, and critical preliminary data for institute operations. Submissions to the Planning track are encouraged in any areas of foundational and use-inspired research appropriate to the program solicitation, NSF, and partner

organizations; this includes all areas of MPS. The following describes some of the opportunities for MPS researchers to partner with researchers in AI and related disciplines to jointly advance both the MPS domain and AI foundations. Teams interested in submitting an AI Research Institute Planning Grant are encouraged to consult the solicitation and discuss their concept with a cognizant Program Director listed below.

MPS encourages planning track proposals that demonstrate how a future AI Research Institute will advance both AI and research domains supported by MPS divisions, including multi-disciplinary proposals with a strong focus on MPS-supported research. Teams are encouraged to consider how their efforts can be amplified through connections to existing cyberinfrastructure, centers, facilities, and institutes.

DIVISION OF ASTRONOMICAL SCIENCES

The exponentially increasing amount of astronomical data requires new approaches that are automated and much more efficient. AI covers a wide range of algorithms, and it is important to navigate this landscape and consider which techniques are most appropriate for which problems. The next generation of astronomers needs to be prepared and ready to embark on research with new AI methods.

DIVISION OF CHEMISTRY

New AI tools that can learn from multi-dimensional data and extrapolate with non-linear predictions have the potential to broadly impact classical chemistry disciplines as well as within interdisciplinary and convergent communities that require a high degree of predictive chemical complexity (e.g. synthetic biology, clean energy, quantum sciences, environmental science, etc.). Beyond accelerating laborious and time-consuming analysis, innovative foundational advances in AI that are inspired by chemical challenges have the potential to provide new perspectives to assist in the discovery of novel trends in structure/property relationships, unprecedented reactivities, and transformative applications. The Division of Chemistry encourages planning proposals to support teams of researchers who will lay the foundation for future institute-level programs aimed towards combining pioneering AI designs for data representation, processing, and prediction with creative approaches for database collection and method testing to achieve ground-breaking advances that overcome chemical and chemistry-related challenges.

DIVISION OF MATHEMATICAL SCIENCES

Rapid development of machine learning technologies and algorithms requires matching advances in building their theoretical underpinnings. Critical questions, such as the interpretability, reliability, and validation of algorithms, need to be addressed before these technologies could have broader and deeper impact on the economy and quality-of-life improvements worldwide.

New mathematical and statistical theories are essential in efficiently dealing with problems of approximation, convergence, optimization in high dimensions that are ubiquitous in machine learning. In light of this, DMS is interested in planning activities that bring together the electrical engineering, mathematics, statistics, and theoretical computer science communities to develop the theoretical foundations of machine learning through integrated research and training activities.

DIVISION OF MATERIALS RESEARCH

AI offers opportunities to accelerate the discovery of new materials and advance challenging scientific problems across the frontiers of materials research. The Division of Materials Research (DMR) welcomes planning activity proposals for an institute that will translate AI research into advances in challenging problems in the domains of DMR's Topical Materials Research Program and Design Materials to Revolutionize and Engineer our Future program, centers, and facilities. In so doing, new directions in AI research will be stimulated. It is important to consider how to meaningfully apply the techniques of machine learning and artificial intelligence in human-interpretable form to materials research and discovery.

The design and discovery of new materials in concert with the goals of the Materials Genome Initiative may be accelerated through the application of artificial intelligence approaches at all stages of the integration of computation, experiment, and theory. Examples might include, but are not limited to, intelligent automation and control of experiments, and the precision synthesis of materials across the scales. AI research may also enhance critical infrastructure for data-intensive materials research, for example, developing intelligent automation to collect, curate, and provenance track materials data and materials knowledge.

Bold and innovative ideas to advance the frontiers of materials discovery and research through the incorporation of AI approaches are particularly welcome in planning for an AI Research Institute focused on advancing the domain-sciences of materials research.

DIVISION OF PHYSICS

Successful Planning Grant proposals for a future AI Research Institute in Physics will provide a roadmap for incorporating novel techniques to accelerate discovery and extend the frontier in AI by addressing research challenges in the domains supported by the Division of Physics. Realizing the full potential of AI for Discovery in Physics will improve the operations and exploitation of Division of Physics facilities, promote the integration and interpretation of heterogenous datasets, accelerate model-building and quantification of uncertainties, and enable novel ways to interrogate high-dimensional features of complex data sets. Planning activities might include workshops, development of partnerships, exploratory collaborative research, and/or engagement of stakeholders that would enhance the integration of AI and Physics communities towards the Institute vision.

POINTS OF CONTACT

AST

- Nigel A. Sharp, Program Director, MPS/AST, (703) 292-4905, email: nsharp@nsf.gov

CHE

- Laura L. Anderson, Program Director, MPS/CHE, (703) 292-8156, email: laanders@nsf.gov
- Jin K. Cha, Program Director, MPS/CHE, (703) 292-2461, email: jcha@nsf.gov
- Katharine Covert, Program Director, MPS/CHE, (703) 292-4950, email: kcovert@nsf.gov

DMR

- Daryl W. Hess, Program Director, MPS/DMR, (703) 292-4942, email: dhess@nsf.gov
- John A. Schlueter, Program Director, MPS/DMR, (703) 292-7766, email: hjschluet@nsf.gov

DMS

- Tomek Bartoszynski, Program Director, MPS/DMS, (703) 292-4885, email: tbartosz@nsf.gov

PHY

- Saul Gonzalez, Program Director, MPS/PHY, (703) 292-2093, email: sgonzale@nsf.gov
- Vyacheslav (Slava) Lukin, Program Director, MPS/PHY, (703 202-7382, email: vlukin@nsf.gov
- Bogdan Mihaila, Program Director, MPS/PHY, (703) 292-8235, email: bmihaila@nsf.gov

National Artificial Intelligence Research Institutes
Program Solicitation: https://www.nsf.gov/publications/pub_summ.jsp?WT.z_pims_id=505686&ods_key=nsf20503

Sincerely,

Anne L. Kinney
Assistant Director, Directorate of Mathematical and Physical Sciences (MPS)