DATA SCIENCE TO ADVANCE CHEMICAL AND MATERIALS SCIENCES

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER: DE-FOA-0002474

Award Selection (August 2021)

The Office of Science of the Department of Energy is pleased to announce that 10 projects (listed below) have been selected to receive funding as part of competition for research in data science, including artificial intelligence (AI) and machine learning (ML), sponsored by the Office of Basic Energy Sciences. The research efforts will advance basic chemical and materials sciences through data-driven models of complex chemical or materials systems whose macroscopic properties depend on collective behavior across multiple time and length scales. These new predictive AI/ML models, validated by experiment, will accelerate discovery of chemical mechanisms, of materials systems with exceptional properties and functionalities, and of novel quantum phenomena. The fundamental knowledge gained will lay a foundation for a wide range of clean energy technologies.

Projects announced at this time are selections for negotiation of financial award. The final details for each award are subject to grant and contract negotiations between DOE and the awardees.

Principal Investigator	Institution	City, State	Proposal Title
Arges, Christopher	Louisiana State University	Baton Rouge, LA	Bridging the length scales in ionic separations via data-driven machine learning
Arnold, Frances	California Institute of Technology	Pasadena, CA	Multimodal approaches for leveraging domain knowledge with state-of-the-art machine learning to engineer biocatalysts
Barros, Kipton	Los Alamos National Laboratory	Los Alamos, NM	Data science driven quantum chemistry for reactive chemistry controlled by stimuli
Chowdhury, Sugata	Howard University	Washington, DC	Machine assisted quantum magnetism
Estroff, Lara	Cornell University	Ithaca, NY	Formulation engineering of energy materials via multiscale learning spirals
Hagan, Michael	Brandeis University	Waltham, MA	Machine learning approaches to understanding and controlling 3D active matter
Ihme, Matthias	Stanford University	Stanford, CA	Integrated data-driven methods for scientific discovery of non-equilibrium thermochemical processes in complex environments from ultrafast x-ray measurements at LCLS
Johnston, Steven	University of Tennessee	Knoxville, TN	Artificial intelligence and data science enabled predictive modeling of collective phenomena in strongly correlated quantum materials
Kozinsky, Boris	Harvard University	Cambridge, MA	Machine learning for accelerated understanding of dynamic catalysis
Robinson, Ian	Brookhaven National Laboratory	Upton, NY	Automated sorting of high repetition rate coherent diffraction data from XFELs