Energy Department to Provide $27.6 Million for Data Science Research in Chemical and Materials Sciences

List of Awards

PI Name	Institution	City, State	Proposal Title
Ceder, Gerbrand	Lawrence Berkeley National Laboratory	Berkeley, CA	Data-Driven Synthesis Science (D2S2)
Najm, Habib	Sandia National Laboratories	Livermore, CA	Machine Learning for Understanding Heavy Hydrocarbon Clustering
Osborn, Raymond	Argonne National Laboratory	Lemont, IL	Structural Signatures of Hidden Order in Spin-Orbit Coupled Systems
Soderholm, Lynda	Argonne National Laboratory	Lemont, IL	Quantifying Energy Drivers in Chemical Separations
Yang, Ping	Los Alamos National Laboratory	Los Alamos, NM	Data-Driven Separation Agent/Solvent Design – An Integrated Simulation-Experiment Approach
Chern, Gia-Wei	University of Virginia	Charlottesville, VA	Machine Learning Aided Modeling of Resistive Switching Phenomena in Correlated Electron Systems
de Hoop, Maarten	Rice University	Houston, TX	DEEP LEARNING FOR FORECASTING OF FRACTURE AND FAULT EVOLUTION
Greeley, Jeffrey	Purdue University	West Lafayette, IN	Data Science-Driven Discovery of Multimetallic Oxygen-Cycle Electrocatalysts for Enhanced Energy Conversion
Gregoire, John	California Institute of Technology	Pasadena, CA	Energy Materials Chemistry Integrating Theory, Experiment and Data Science
Hirschfeld, Peter	University of Florida	Gainesville, FL	Data-science enabled discovery of superconductors
Huang, Pinshane	University of Illinois	Champaign, IL	Massive all-atom analysis of 2D materials with quantum properties
Isborn, Christine	University of California - Merced	Merced, CA	Applying Deep Learning Methods to Develop New Models of Charge Transfer, Nonadiabatic Dynamics, and Nonlinear Spectroscopy in the Condensed Phase
Jacobs, Ryan	University of Wisconsin - Madison	Madison, WI	Leveraging High-throughput Computation and Machine Learning to Discover and Understand Low-Temperature Fast Oxygen Conductors
Janik, Michael	Pennsylvania State University	University Park, PA	Data-driven discovery of intermetallic catalysts with controlled active site nuclearity
Kitchin, John	Carnegie Mellon University	Pittsburgh, PA	Data-directed synthesis of multicomponent materials for light-driven hydrogen production from oxygenates

PI Name	Institution	City, State	Proposal Title
Krause, Amanda	University of Florida	Gainesville, FL	Elucidating Grain Growth in Thermo-Magnetic Processed Materials by Transfer Learning and Reinforcement Learning
Molinero, Valeria	University of Utah	Salt Lake City, UT	Elucidating the formation mechanisms of zeolites using data-driven modeling and in-situ characterization
Schuh, Christopher	Massachusetts Institute of Technology	Cambridge, MA	Discovery and Design of Stable Nanocrystalline Alloys: The Grain Boundary Segregation Genome
Wang, Qi	University of South Carolina	Columbia, SC	Data-science enabled investigation of the mechanisms for multiscale ion transport in functional electrolytes and for the radical generation in crystalline assemblies