THE CAMILLE AND HENRY DREYFUS FOUNDATION, INC.

Machine Learning in the Chemical Sciences and Engineering Awards

Institution	Awarde	Project
2022		
Cornell University	Robert DiStasio	Semi-Local Density Fingerprints for Machine Learning Molecular Properties, Intra-/Inter-Molecular Interactions, and Chemical Reactions
Cornell University	Julia Dshemuchadse	Discovery of New Self-Assembled Crystal Structures for Materials Design
Harvard University	Boris Kozinsky	Learning non-local functionals and equivariant models for reactive dynamics
Massachusetts Institute of Technology	Stephen Leffler Buchwald	Active Scientific Machine Learning of Chemical Reaction Networks and Chemical Reactivity in Transition Metal Catalysis
New York University	Mark Tuckerman	Machine learning the theorems of density functional theory
University of Chicago	Gregory A. Voth	Physics-Constrained Machine Learning for Reactive Molecular Dynamics
University of Michigan, Ann Arbor	Wenhao Sun	Machine-Learning Classification of Materials Synthesizability
University of Utah	Connor Bischak	Uncovering Structure-Function Relationships in Organic Mixed Conductors: High-Throughput Electrochemistry Guided by Machine Learning
2021		
Boston University	Qiang Cui	Understanding Protein Allostery using Machine Learning and Deep Mutation Data
California Institute of Technology	Garnet Chan	New Opportunities for Machine Learning in Quantum Chemistry
Massachusetts Institute of Technology	Rafael Gomez-Bombarelli	Adversarial Attacks on Interatomic Potentials for Active Learning and Inverse Design
North Carolina State University	Milad Abolhasani	An Autonomous Robo-Fluidic Microprocessor: Machine Learning-Guided Synthesis Process Development of Quantum Dots
Princeton University	Abigail Doyle	Artificial Intelligence for Chemical Reaction Prediction
University of Illinois at Urbana-Champaign	Nicholas Jackson	Machine Learning Quantum Chemistry Over Coarse-Grained Fields
University of Michigan	Sriram Chandrasekaran	Predicting Moonlighting Metabolic Regulators Using Mechanistic Deep Learning
2020		
California Institute of Technology	Frances H. Arnold	Validation and Dissemination of Machine Learning-Assisted Enzyme Engineering
California Institute of Technology	Thomas F. Miller	Molecular-Orbital-Based Machine Learning for Excited States
California Institute of Technology	John H. Seinfeld	Application of Machine Learning to Represent the Molecular Routes Comprising Atmospheric Chemistry
Massachusetts Institute of Technology	Klavs F. Jensen	Machine-Learning-Guided Discovery of New Electrochemical Reactions.
Purdue University	Brett M. Savoie	Transfer Learning for Deep Generative Chemical Models
The University of Chicago	Andrew L. Ferguson	Data-driven Protein Engineering Using Deep Generative Learning and High-throughput Gene Synthesis
Tufts University	Yu-Shan Lin	Low-supervision Machine Learning for Automated Analysis of Molecular Dynamics Simulations
University of Minnesota	Jason D. Goodpaster	Machine Learning Models for Chemical Reactions