

Machine Learning in the Chemical Sciences and Engineering Awards

2021

North Carolina State University
Machine Learning-Guided Synthesis Process Development of Quantum Dots

Milad Abolhasani

California Institute of Technology
New Opportunities for Machine Learning in Quantum Chemistry

Garnet Chan

University of Michigan
Predicting Moonlighting Metabolic Regulators Using Mechanistic Deep Learning

Sriram Chandrasekaran

Boston University
Understanding Protein Allostery using Machine Learning and Deep Mutation Data

Qiang Cui

University of California, Los Angeles
Artificial Intelligence for Chemical Reaction Prediction

Abigail Doyle

Massachusetts Institute of Technology
Adversarial Attacks on Interatomic Potentials for Active Learning and Inverse Design

Rafael Gomez-Bombarelli

University of Illinois at Urbana-Champaign
Machine Learning Quantum Chemistry Over Coarse-Grained Fields

Nicholas Jackson

2020

California Institute of Technology
Validation and Dissemination of Machine Learning-Assisted Enzyme Engineering

Frances Arnold

The University of Chicago
Data-driven Protein Engineering Using Deep Generative Learning and High-throughput Gene Synthesis

Andrew Ferguson

University of Minnesota
Machine Learning Models for Chemical Reactions

Jason Goodpaster

Massachusetts Institute of Technology
Machine-Learning-Guided Discovery of New Electrochemical Reactions

Klavs Jensen

Tufts University
Low-supervision Machine Learning for Automated Analysis of Molecular Dynamics Simulations

Yu-Shan Lin

California Institute of Technology
Molecular-Orbital-Based Machine Learning for Excited States

Thomas Miller

Purdue University
Transfer Learning for Deep Generative Chemical Models

Brett Savoie

California Institute of Technology
Application of Machine Learning to Represent the Molecular Routes Comprising Atmospheric Chemistry

John Seinfeld