

Dr. Nicholas Jackson

Assistant Scientist

Center for Molecular Engineering & Materials Science Division
Argonne National Laboratory

Thursday, December 12, 2019, 3:30 – 4:30 pm
Armstrong Hall of Engineering, Room B071

Charge-Functional Polymer Design at the Nexus of Multiscale Modeling and Machine Learning



Dr. Jackson obtained his BA in Physics from Wesleyan University (2011) studying semi-classical vortex drag in superfluid Helium II with Professor Fred Ellis. Nick then joined the groups of Prof. Mark Ratner and Prof. Lin Chen at Northwestern University, where he received his PhD in Theoretical and Computational Chemistry (2016) studying optoelectronic processes in semiconducting polymers and small molecules. In 2016, Nick began a post-doc with Prof. Juan de Pablo at the University of Chicago, and subsequently accepted a Maria Goeppert Mayer Fellowship at Argonne National Laboratory, where he worked on multiscale simulations of molecular and polymeric interfaces, machine-learning enhanced simulation methodologies, and data-enabled soft materials design. Currently, he is an Assistant Scientist in the Materials Science Division at Argonne National Laboratory.

Abstract: In the past century, tailoring the mechanical properties of polymers transformed the economies of the world. In the next century, tailoring the charge-functional properties of soft materials (e.g. electronic and ionic conduction) has the potential to do the same. In this talk, I will outline the landscape of soft materials modeling and the crucial role that the integration of theory, simulation, and data science play in enabling the design and understanding of charge-functional polymers. Specifically, I will focus on the application of machine learning to i) enable the mapping of *ab-initio* quality electronic structure to coarse-grained models of conjugated polymers and ii) design sequence-specific polymer architectures with targeted structural properties. I will conclude with a vision for soft materials research that holistically combines machine learning and data science with multiscale modeling to design soft materials with desirable bioelectronic, static electrical, and adhesive properties.