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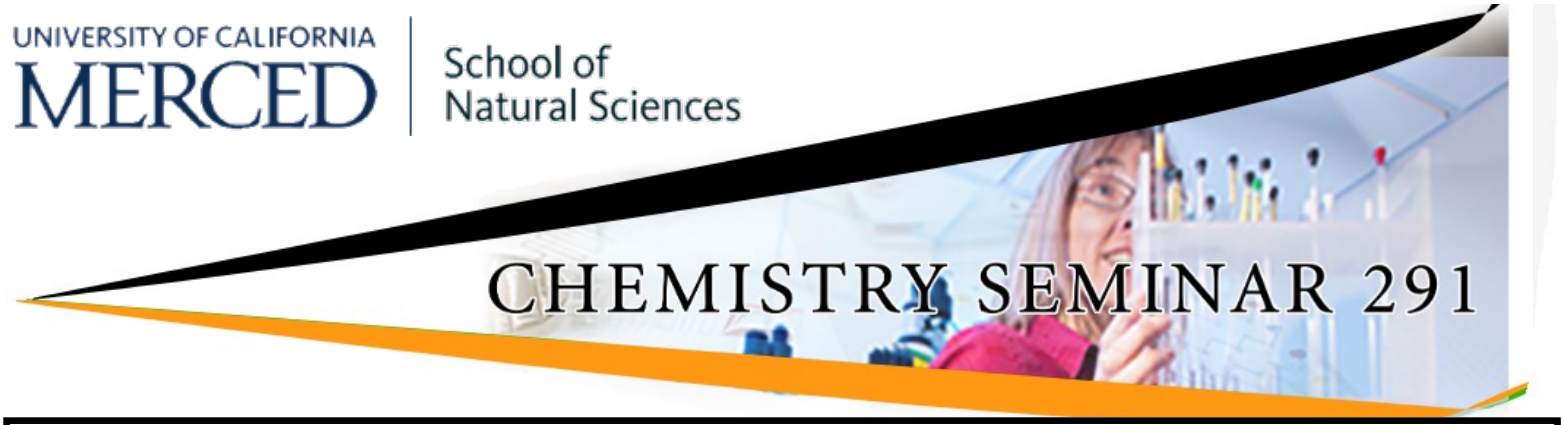

Molecular Design Blueprints: Materials and Catalysts from New Simulation and Machine Learning Tools

Date: **1/31/2020**

Time: **3:00 - 4:20 PM**

Location: **COB1 267**

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Abstract

Many compelling functional materials and highly selective catalysts have been discovered that are defined by their metal-organic bonding. The rational design of de novo transition metal complexes however remains challenging. First-principles (i.e., with density functional theory, or DFT) high-throughput screening is a promising approach but is hampered by high computational cost, particularly in the brute force screening of large numbers of ligand and metal combinations. In this talk, I will outline our efforts over the past few years to accelerate the design of inorganic complexes for catalysis and materials science: i) We have automated and simplified simulation, eliminating the need for tedious manual preparation of computational chemistry calculations, ii) We developed machine learning (ML) models that predict properties in a fraction of the time of traditional calculations, iii) We developed ML models that can predict outcomes of simulations for dynamic, autonomous control, and iv) We integrated these tools into an automated design workflow for the evolutionary algorithm optimization of materials properties with awareness of ML model and DFT model uncertainty. I will describe how this powerful toolkit has advanced our understanding of a range of metal-organic complexes from functional spin crossover materials to open-shell transition metal catalysts by enabling the rapid screening of thousands of candidate molecules and by revealing robust design rules.

About the Speaker

Professor Heather J. Kulik is an Associate Professor in the Department of Chemical Engineering at MIT. She received her B.E. in Chemical Engineering from the Cooper Union in 2004 and her Ph.D. from the Department of Materials Science and Engineering at MIT in 2009. She completed post-doctoral training at Lawrence Livermore and Stanford, prior to joining MIT as a faculty member in November 2013. Her research has been recognized by a Burroughs Wellcome Fund Career Award at the Scientific Interface, Office of Naval Research Young Investigator Award, DARPA Young Faculty Award, NSF CAREER Award, the AAAS Marion Milligan Mason Award, and the Journal of Physical Chemistry Lectureship, among others.