ETH zürich

Department of Mechanical and Process Engineering
Institute of Energy and Process Engineering

IEPE Seminar Series

What problems can machine learning solve in transition metal complex discovery?

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 to accelerate the design of inorganic complexes for catalysis and materials science applications: i) We automated and simplified simulation in transition metal chemistry, overhauling the previous tedious manual approach, 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 and suitability of methodology 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 metal-organic bonding in materials far-ranging from functional spin crossover complexes to open-shell transition metal catalysts and metal-organic frameworks by enabling the rapid screening of millions of candidate molecules and by revealing robust design rules.

Prof. Heather J. Kulik – MIT

Biography: 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 postdoctoral 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, DARPA Director's fellowship, NSF CAREER Award, the AAAS Marion Milligan Mason Award, the Journal of Physical Chemistry Lectureship, and a Sloan Fellowship in chemistry, among others.

Friday, 09. April 2021 **16h00–17h00** **Zoom**

Meeting ID: 667 4760 5485
Password: 130034

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