Professor Heather J. Kulik is an assistant professor in the Department of Chemical Engineering at the Massachusetts Institute of Technology (MIT). She received her bachelor's degree in Chemical Engineering from the Cooper Union for the Advancement of Science and Art in 2004, and her doctorate from the Department of Materials Science and Engineering at MIT, in the group of Nicola Marzari in 2009. She completed post-doctoral training in the group of Felice Lightstone at the Lawrence Livermore (2010) and Todd J. Martinez at Stanford (2010−13), prior to joining MIT as a faculty member in November 2013. Her research in accelerating computational modeling in inorganic chemistry and catalysis 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, and the AAAS Marion Milligan Mason Award, among other awards.

Chemical space is vast, with best estimates suggesting we have as yet characterized less than 1 part in 10^50 of all possible compounds. The need for efficient discovery of new materials and catalysts mandates that we identify smart ways to map out and explore chemical space. Virtual high throughput screening, typically driven by first-principles, density functional theory (DFT) calculations, has emerged as a powerful tool for the discovery of new materials. I will describe our recent development of the first open source toolkit for inorganic molecular discovery, molSimplify. i) We introduce a first-of-its-kind divide-and-conquer approach to generate precise geometries of new inorganic complexes for automated simulation and characterization with DFT. ii) We leverage multimillion-molecule organic libraries for inorganic discovery that ensure stable building blocks while maximizing molecular diversity to provide efficient traversal of chemical space. iii) We train machine learning models (e.g., neural networks and kernel ridge regression models) to predict quantum mechanical properties in seconds for use in efficient screening workflows as opposed to minutes or hours with DFT. iv) We develop automated strategies to uncover structure-property correlations for design. I will describe how implementing all of these techniques in our open source toolkit has advanced applications in quantum dot synthesis for materials science and catalyst design for selective, direct conversion of methane to methanol.

Open Forum: 4:30-5:30 p.m. Tuesday, Jan. 29
Kate & Michael Bárány Conference Room (117/119 Smith Hall)
Women in STEM

Host: Professor Jason Goodpaster
Refreshments will be served prior to the seminar.
Visit: chem.umn.edu/chemistry-events for a schedule of upcoming seminars.