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Discovering Tunable Materials with Unprecedented Properties Using High-Throughput Quantum Chemistry

Monday July 11th
Lecture 4:00-5:00 p.m. | Physics/Astronomy Auditorium (PAA) A118
Reception 5:00-6:00 p.m. | Benson Hall Lobby

Bio

Andrew Rosen is a Miller Research Fellow at the University of California, Berkeley hosted by Prof. Kristin Persson. His research is focused on using computational methods and the fundamental principles of quantum mechanics to accelerate the discovery of novel materials that can address global challenges in energy, sustainability, and the chemical industry. Andrew completed his Ph.D. in Chemical Engineering at Northwestern University with Prof. Randall Snurr and Prof. Justin Notestein where he studied redox processes in metal–organic frameworks. Beyond his current role as a Miller Fellow, Andrew has been named an American Chemical Society CAS Future Leader, a National Defense Science and Engineering Graduate Fellow, a Ryan Fellow of the International Institute for Nanotechnology, and a Presidential Fellow – the highest honor awarded to graduate students at Northwestern. Andrew is particularly passionate about accessible and equitable education in chemical engineering, for which he has received several teaching and mentorship awards. Originally from New York, Andrew pursued his B.S. in Chemical Engineering at Tufts University before making his westward journey across the states. His favorite molecule is the buckyball C_{60}.

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Abstract

The solutions to many of society's most pressing problems rely on the discovery of materials with optimal properties that are unique to the application of interest. In many cases, it is not a matter of incremental improvement over existing technologies; rather, it is a need to identify new kinds of materials altogether. This is especially the case in the areas of energy and sustainability where transformational changes often remain the only viable path forward. The conventional trial-and-error approach of materials discovery, however, can be extremely time-consuming and rarely identifies optimal candidates, especially when they exist beyond the limits of our current chemical intuition.

In this talk, I will discuss how quantum chemistry, high-throughput computing, and machine learning can accelerate the discovery of novel materials to address a variety of global challenges relevant to the field of chemical engineering. Specifically, I will focus on the computationally guided design of synthetically tunable solid-state materials — ones in which the atomistic and/or electronic structure can be precisely controlled and subsequently tailored for a given application.

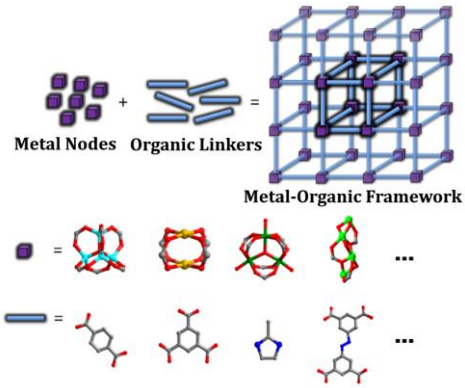

Figure 1. Illustration of a MOF structure, highlighting how metal nodes and organic linkers can yield a crystalline framework composed of unique building blocks.

As one example of this approach from my research, I will highlight recent work involving a relatively new class of materials known as metal–organic frameworks (MOFs), which are porous solids with atomically defined structures composed of metal clusters ("nodes") connected by organic molecules ("linkers"), as depicted in Figure 1. By leveraging the fundamental principles of quantum mechanics, I have developed a computational screening workflow that can automatically predict a wide range of physical and chemical properties for thousands of MOFs in a matter of days, whereas it can often take months to synthesize and test even a single new MOF in the lab. I will share several examples where this unique workflow has been used to discover novel MOFs for heterogeneous catalysis, industrial gas separations, and next-generation electronic devices as it relates to the more efficient production of valuable chemical products.

With recent advances in big data and machine learning in mind, I will also discuss my recent work involving the Materials Project (www.materialsproject.org), which provides public access to predicted properties for nearly all inorganic compounds as well as over 20,000 MOFs via the new Quantum MOF Database that I have developed (Figure 2). To conclude, I will provide a brief outlook on some of the opportunities and grand challenges in the area of computational materials discovery for chemical engineering.

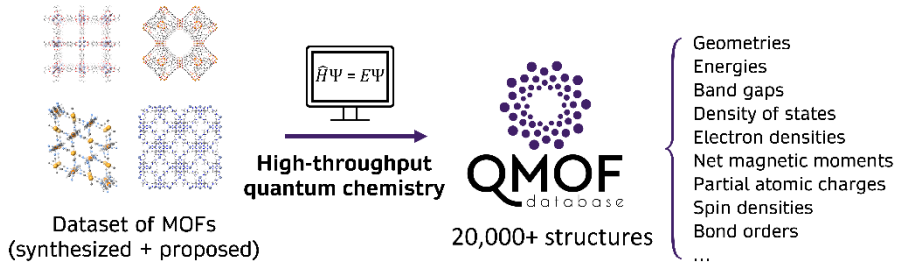

Figure 2. Overview of the Quantum MOF (QMOF) Database, which you can explore on the Materials Project at www.materialsproject.org/mofs.