UC San Diego
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UCSD NANO & CHEMICAL ENGINEERING

SPECIAL SEMINAR

February 23rd 2023

Seminar Presentation: 9:30am – 10:30am

SME Room 248

"Discovering Tunable Materials with Unprecedented Properties via High-Throughput Quantum Chemistry"

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Abstract: The solutions to many of society's most pressing problems rely on the discovery of materials with unprecedented physical and chemical properties that are tailored to an application of interest. Typically, it is not a matter of incremental improvements over existing technologies; rather, there is often an urgent need to identify new kinds of materials altogether. The conventional trial-and-error approach of experimental materials discovery, however, can be extremely time-consuming and may not identify truly top-performing candidates, particularly 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 help guide experiments and accelerate the discovery of novel materials to address a variety of global challenges relevant to the field of chemical engineering. To demonstrate the impact and versatility of this approach, I will highlight how a novel computational screening platform that I developed can drastically accelerate the discovery of porous framework solids for heterogeneous catalysis, industrial gas separations, and next-generation (opto)electronic devices as it relates to the more sustainable production of valuable chemical products. With advances in data science in mind, I will also discuss my recent work building upon the Materials Project — a publicly accessible database of computed physicochemical properties for over 100,000 solid-state materials — and how such a resource can aid both theorists and experimentalists in the design of materials with targeted electronic properties. Overall, this work demonstrates how high-throughput virtual screening methods rooted in the fundamental principles of quantum mechanics have set the stage for autonomous materials discovery platforms of the future.

Educational Development and Training: Outside of research, Andrew is also particularly passionate about accessible and equitable education in engineering. For over a decade, he has run a website called "Rosen Review" where he shares accessible STEM education resources with the global community, particularly with a focus on topics in chemical engineering. This resource that has been viewed by over one million people from nearly every country around the world. At Northwestern, Andrew co-led the Chemical and Biological Engineering Teaching Committee, which is a student-run organization dedicated to sharing inclusive teaching practices from the STEM education literature. Andrew is also regularly engaged in research within the area of data analytics and teaching; he has previously published a paper on the topic of trends and biases in student evaluations of teaching, which has since become a widely cited resource in the community.

Biosketch: Dr. Andrew Rosen is a Miller Research Fellow at the University of California, Berkeley where his research has focused on uncovering unique electronic structure properties in solid-state materials as part of the Materials Project team led by Prof. Kristin Persson. Andrew earned his Ph.D. in Chemical Engineering at Northwestern University where he studied redox processes in metal–organic frameworks in the groups of Prof. Randall Snurr and Prof. Justin Notestein. Beyond his current role as a Miller Fellow, Andrew has been named a CAS Future Leader by the American Chemical Society, a National Defense Science and Engineering Graduate Fellow, a Ryan Fellow of the International Institute for Nanotechnology, and a Presidential Fellow of Northwestern University.