

Machines Meet Materials: Challenges and Opportunities in Discovery and Design

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**Chemistry
Seminar on the
use of Machine
Learning in
Materials
discovery**

**Monday
Oct 12 at 4
pm in 126
Schrenk**

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Abstract: The deployment of beyond-lithium-ion battery technologies for portable and stationary grid energy-storage applications is limited by the challenge of discovering and designing novel high-energy-density cathode-active materials (CAMs) within the vast materials space.

The first part of this talk delves into establishing a scalable, transferable framework for accelerating the discovery of stable, high-energy-density CAMs for sodium-ion batteries (SIBs) by integrating techniques from the computational materials science toolbox. I will introduce a scalable, data-driven framework for discovering robust SIB cathodes by integrating large-scale data (> 5 million materials), descriptor-based machine learning (ML), and first-principles validation. This large-scale ML-integrated framework significantly reduces reliance on expensive first-principles calculations while uncovering chemical and structural trends that govern high-voltage performance. The current workflow, however, is limited to discovering existing materials. In the second part, I will discuss how one can extend the present framework to the inverse design of new materials by integrating chemistry-aware structure generation and reinforcement learning.

About the speaker: Dr. Mohammad R. Momeni obtained his Ph.D. in Theoretical and Computational Chemistry from the University of Alberta, Canada. Later, he held three postdoc appointments at the University of Minnesota, UC San Diego, and NJIT, where he studied the structure and dynamics of metal-organic frameworks, guest-molecule adsorption, heterogeneous catalysis, and vibrational spectroscopy. Currently, he is an assistant professor at UMKC, and his research interests are interdisciplinary, encompassing Theoretical Chemistry and Physics and Materials Science. He is broadly interested in developing multiscale classical and quantum path-integral simulation techniques, new algorithms for studying the dynamics and spectroscopy of condensed-phase and interface systems, and advancing the design and discovery of new materials for applications in sustainable energy conversion and storage. Over the past ~20 years of active research, he has published a book chapter on photovoltaics and authored/co-authored more than 50 articles in peer-reviewed journals. Dr. Momeni is one of the leading developers of the general-purpose MD software package DL_POLY Quantum (<https://github.com/mrmomeni>).