Dear Colleagues & Students,

You are cordially invited to a special seminar

Atomistic and generative modeling for material design and synthesis prediction

Presented by:

Dr. Peichen Zhong

Department of Materials Science and Engineering,

National University of Singapore

Date: **4th Jun 2026, Thursday** Time: **10:00am-12:00pm**

(Light refreshments will be provided before the seminar.)

Venue: **Block EA, level 6, EA-06-03 (NUS Campus Map)**

Hosted by: **Associate Professor Daria Andreeva-Baeumler**

Abstract:
Atomistic simulation has become an indispensable tool in computational materials science, enabling property predictions and mechanistic insights across a wide range of chemical and structural environments. While recent advancements in artificial intelligence (AI), such as machine learning interatomic potentials (MLIPs), have significantly expanded the spatial and temporal scales of these simulations, exploring high-dimensional chemical spaces with quantum-level accuracy remains computationally demanding. Simultaneously, the emergence of generative modeling has demonstrated the potential to revolutionize computational materials chemistry.
In this presentation, I will discuss a diffusion-based deep generative model (CHGGen) that integrates inpainting generation and foundation potential optimization for crystal structure prediction. I will demonstrate how this model elucidates atomic configurations and Li transport properties in crystalline and amorphous $LiPO_2F_2$ (LiDFP), and explain why amorphous LiDFP can be stabilized within the solid-electrolyte interphase (SEI). Finally, I will discuss a thermodynamic criterion for evaluating solid-state synthesizability beyond the widely used 0 K energy above the convex hull, aiming to close the AI materials synthesizability gap.

Biography:
Dr. Peichen Zhong is an Assistant Professor at the Department of Materials Science and Engineering, National University of Singapore. He obtained a BS in Physics from the University of Science and Technology of China (USTC) in 2018, followed by a PhD in Materials Science from UC Berkeley in 2023. He then completed the postdoctoral work at Lawrence Berkeley National Laboratory (LBNL) and Bakar Institute of Digital Materials for the Planet (BIDMaP). He was awarded the 2023 Rising Stars in Materials Science and Engineering by CMU/MIT/Stanford, the BIDMaP Emerging Scholar Fellowship from the College of Data Science, Computing and Society (CDSS) at UC Berkeley, and the AI2050 Early Career Fellowship by Schmidt Sciences. Dr. Zhong leads the Applied Machine Learning and Materials Modeling (AM3) Group at NUS MSE. The AM3 Group focuses on both methodology development and the material application to pioneer advanced technologies.

Looking forward to seeing all of you!