

Physical Chemistry Seminar

Jake Vu

Graduate Student | The Chen Group | Purdue University

Modeling Complex Material Systems: From Physics to AI

Modeling complex material systems remains challenging because the relevant phenomena span multiple levels of theory, from quantum mechanical descriptions of electrons to large configurational spaces of atomic structures. This talk presents a progression of computational approaches aimed at improving the accuracy and efficiency of simulations in regimes where traditional methods become impractical. We begin at the electronic structure level, focusing on extreme environments such as warm dense matter, where conventional density functional theory becomes computationally prohibitive. To address this challenge, we employ stochastic density functional theory (sDFT) with noise-reduction techniques to enable linear-scaling simulations of metallic systems at finite temperatures. We then move to atomistic modeling of deep-Earth materials, where strong anharmonic lattice dynamics cannot be accurately captured by classical force fields. In this regime, machine-learned interatomic potentials trained on ab initio data provide an efficient framework for modeling anharmonic behavior while keeping near first-principles accuracy. Finally, we explore generative modeling for catalytic surfaces, introducing a diffusion-based approach augmented with a physics-guided drift term to steer sampling toward physically meaningful configurations. Applications to surfaces such as Ag(111) and Pd(111) demonstrate how generative models can efficiently find representative catalytic structures. Together, these examples illustrate how physics-based modeling and modern AI methods can be integrated to expand the scope of computational materials research.