



Department of Materials Science
& Engineering
College of Design and Engineering

▶ Department Seminar

From Quantum Chemistry to Materials Design: Bridging Scales with AI

Date: 19 Oct 2026 (Monday)

Time: 11:00 AM – 11:59 AM

Venue: EA LT7A, Level 1



Dr. Wen YAN

Head of Research: AI for Science
ByteDance Seed

Abstract

Connecting electronic structure to macroscopic properties is a central challenge in computational materials science. This seminar presents our team's efforts to bridge these scales through advances in quantum chemistry, molecular simulation, and artificial intelligence. Topics include accelerated electronic structure calculations, quantum-mechanical datasets, and learned interatomic potentials and polarizable force fields for organic liquids and battery electrolytes. These developments provide a foundation for generative electrolyte design, where molecular modeling guides the discovery and experimental evaluation of new formulations. A brief discussion of protein–ligand binding free energies and molecular sampling will illustrate connections to biological applications. The talk will emphasize the physical principles underlying these approaches and the open challenges in achieving accurate, transferable, and computationally efficient predictions.

Biography

Wen Yan is a research scientist at ByteDance, where he combines machine learning and molecular simulation to address problems in materials science and biology. He previously worked at the Flatiron Institute (2016–2022), developing computational and mathematical methods for soft and active matter. He received his PhD from the California Institute of Technology in 2016.

Looking forward to seeing all of you!

Hosted by: Peichen Zhong