MM 2: Invited Talk: Richard Hennig

Time: Monday 9:30–10:00 Location: SCH/A251

Invited Talk MM 2.1 Mon 9:30 SCH/A251

Deep-Learning and Generative AI for the Discovery of Electron-Phonon Superconductors — •Richard Hennig — University of Florida, Gainesville, Florida, USA

The search for new superconductors with higher critical temperatures, T_c, and critical fields, H_c, is limited by the cost of electron-phonon calculations and the vastness of compositional and structural space. To overcome both obstacles, we develop an integrated deep-learning workflow for conventional, electron-phonon-mediated superconductors.

First, we introduce BEE-NET, an ensemble of equivariant graph neural networks trained to predict the Eliashberg spectral function $\alpha^2F(\omega)$ and T_c directly from crystal structures, optionally augmented by the phonon density of states. Unlike traditional approaches that learn T_c directly, predicting $\alpha^2F(\omega)$ treats superconductors and non-superconductors on equal footing and, together with explicit phonon-spectrum information, leverages electron-phonon physics to improve predictions for rare superconducting materials. Embedded in a multi-stage screening pipeline that combines elemental substitution strategies with machine-learned interatomic potentials, BEE-NET scans over 1.3×10^6 candidate structures and down-selects to 741 dynamically and thermodynamically stable compounds with DFT-confirmed $T_c > 5$ K, including two experimentally realized new superconductors.

Finally, I will briefly show how guided diffusion models for crystal structures and our Open Materials Generation (OMatG) framework based on stochastic interpolants extend this physics-informed, data-driven approach to the generative design of new superconductors.