Kyle Michel

Session 3

Bio: Kyle Michel is a software engineer at Meta working on AI-accelerated materials discovery on the FAIR (Fundamental AI Research) Chemistry team. He currently leads development of materials workflows and job orchestration across HPC clusters and public and private clouds. His prior work spans first-principles materials simulation (PhD from UCLA and postdoc at Northwestern), development of AI platforms for materials and chemicals companies (cofounder and CTO of Citrine Informatics), and real-time data systems (tech lead at Nike).

Title: AI-Accelerated Materials Discovery at Meta

Abstract: Advancement of key technologies is often limited by the availability of materials possessing some combination of required properties. Discovery of new materials that satisfy these requirements involves the exploration of massive compositional and structural design spaces. First-principles methods can give accurate predictions of these material properties but require significant computational resources. The field of materials discovery is rapidly adopting AI models that can supplement or replace first-principles methods at a fraction of the cost, allowing for the screening of several orders-of-magnitude more materials systems than would otherwise be possible. This talk will highlight two areas of materials discovery that Meta is in a unique position to contribute back to the community: generation of massive simulation datasets using a combination of HPC clusters and public and private clouds; and state-of-the-art AI models for the prediction of materials properties at the atomic scale. The effectiveness of this work will be demonstrated with real examples of open science materials design workflows at Meta.