Frontier Chemistry Center
フロンティア化学教育研究センター

講演会

演 題：Computational materials discovery in the age of machine learning

講 師：Prof. Chris Bartel
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日 時：2025 年 8 月 28 日（木）14:45~15:45

場 所：北海道大学工学部 材料・化学系棟 MC208

Abstract: Quantum chemical calculations using density functional theory (DFT) are now commonplace in solid-state chemistry. There are several publicly available materials databases (e.g., Materials Project) that house DFT calculation results for millions of inorganic crystals, providing an excellent starting point for finding new materials with interesting properties. High-throughput computational screening of materials using DFT is now being augmented and accelerated using machine learning (ML). In this talk, I'll discuss some shortcomings in the "early days" of ML-driven materials discovery (circa 2021) before transitioning to state-of-the-art approaches. Modern approaches leverage universal machine learning interatomic potentials along with generative artificial intelligence to rapidly search materials space. We have recently been working to establish baselines for these approaches to better understand their advantages and disadvantages compared with more traditional materials discovery methods (e.g., ionic substitutions in known crystals). This talk will also discuss our work towards a new frontier for ML applications in solid-state chemistry, which is to predict and learn from the DFT-calculated electron density.

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