Physikalisches Kolloquium

Universität Konstanz

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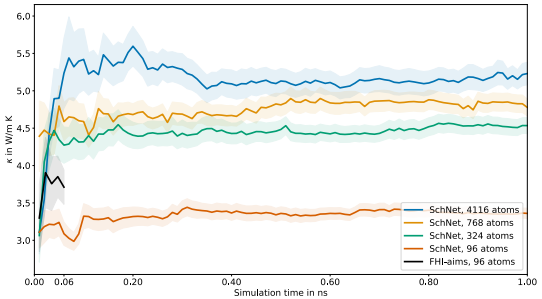

Machine Learning for Quantum Mechanics: Fast Accurate Interpolation of Electronic Structure Calculations

The computational study of atomistic systems has become an essential tool for physics, chemistry, and materials science but is often limited by the high computational cost of first-principles calculations. Data-driven surrogate models, trained on a few selected reference calculations, can accurately interpolate between these at a fraction of the computational cost. Effectively, this maps the problem of solving a complex equation such as the electronic Schrödinger equation for many related systems onto a non-linear statistical regression problem. This approach can yield orders-of-magnitude improvements in system sizes, simulation lengths, and numbers of systems that can be treated, enabling new insights and applications. Key examples include large-scale exploration of chemical and materials spaces for discovery, study, and design of molecules and materials; simulating large atomistic systems over long time scales; and accurate and precise property predictions. I will provide an introduction to this area, emphasizing distinctive traits of this setting and the role of domain knowledge, and present some of our current projects. These include rigorous model assessment, "ultra-fast" machine-learning potentials, message-passing neural networks for Green-Kubo thermal conductivities, and an outlook on surrogate models for quantum Monte Carlo calculations.