Stuttgarter Physikalisches Kolloquium

Fachbereich Physik, Universität Stuttgart
Max-Planck-Institut für Festkörperforschung
Max-Planck-Institut für Intelligente Systeme

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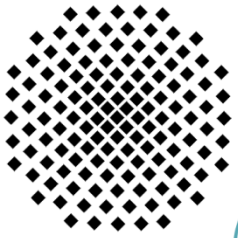

Dienstag, 29. April 2025	16:15 Uhr	V57.02

Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart-Vaihingen

Gastgeber: Prof. Dr. Christian Holm, Universität Stuttgart, Telefon: 0711 - 685-63701

Between physics and scaling: inductive biases in atomistic machine learning

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Abstract

Machine-learning techniques are often applied to perform "end-to-end" predictions, making black-box estimates of a property of interest using only a coarse description of the corresponding inputs. In contrast, atomic-scale modeling of matter is most useful when it allows one to gather a mechanistic insight into the microscopic processes that underlie the behavior of molecules and materials.

In this talk I will provide an overview of the progress that has been made combining these two philosophies, using data-driven techniques to build surrogate models of the quantum mechanical behavior of atoms, enabling "bottom-up" simulations that reveal the behavior of matter in realistic conditions with uncompromising accuracy. I will critically discuss two ways by which physical-chemical ideas can be integrated into a machine-learning framework. One way involves using physical priors, such as smoothness or symmetry of the structure-property relations, to inform the mathematical structure of a generic ML approximation - an approach that has become ubiquitous in the field, but that is increasingly challenged by the emergence of unconstrained models that can directly learn physical constraints from large amounts of data. The other entails a deeper level of integration, in which explicit physics-based models and approximations are built into the model architecture. I will discuss several examples of the application of these ideas, from the calculation of electronic excitations to the design of solid-state electrolyte materials for batteries and high-entropy alloys for catalysis, emphasizing both the accuracy and the interpretability that can be achieved with a hybrid modeling approach, and providing an overview of the exciting research directions that are made available by these new modeling tools.