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Machine learning at the atomic scale: from structural representations to chemical insight

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Abstract

When modeling materials and molecules at the atomic scale, achieving arealistic level of complexity and making quantitative predictions areusually conflicting goals. Data-driven techniques have made great strides towards enabling simulations of materials in realistic conditions with uncompromising accuracy.

In particular, statistical regression techniques have become very fashionable as a tool to predict the properties of systems at the atomicscale, sidestepping much of the computational cost of accurate quantum chemical calculations, and making it possible to perform simulations thatrequire thorough statistical sampling without compromising on the accuracyof the electronic structure model.

I will show that data-driven modelling can be rooted in a mathematically rigorous and physically-motivated symmetry-adapted framework, and discussthe benefits of taking a well-principled approach.

I will present several examples demonstrating how the combination ofmachine-learning and atomistic simulations can offer useful insights on thebehavior of complex systems, and discuss the challenges towards an integrated modeling framework in which physics-driven and data-driven steps can be combined to improve the accuracy, the computational efficiency andthe transferability of predictions, from interatomic potentials toelectronic-structure properties.