

SYMMETRY MATTERS: LEARNING SCALARS AND TENSORS IN MATERIALS AND MOLECULES

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A key problem in atomistic modelling is the determination of the properties of molecules and condensed phases, from stabilities through forces to electric response tensors. This problem underpins our understanding of chemical and material systems and their transformations.

I will show that a machine-learning model based on a local description of chemical environments and Bayesian statistical learning provides a unified framework to predict scalar as well as tensorial atomic-scale properties. This model captures the quantum-mechanical effects that govern the complex surface reconstructions of silicon, predicts the stability of different classes of molecules with chemical accuracy, and distinguishes active and inactive protein ligands with more than 99% reliability. It can also be extended to learn tensorial properties without needing to explicitly define a local reference frame, using a symmetry adapted approach: this allows the prediction of electric response tensors and charge densities.

The universality and systematic nature of this framework provides new insight into the potential energy surface and multipole moment surfaces of materials and molecules.