MAR17-2016-009506

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Many-Body Tensor Representation for Machine Learning of Materials

MATTHIAS RUPP, Fritz Haber Institute of the Max Planck Society

Computational discovery and design of novel materials requires large numbers of accurate electronic structure calculations, whose high computational cost is a limiting factor. Machine learning can significantly reduce the number of necessary calculations by interpolating between a set of reference calculations. For this, a numerical representation of atomistic systems that supports interpolation is crucial. We present a many-body tensor representation that can encode both molecules and crystals, has proper mathematical structure, is invariant to translation, rotation, and nuclear permutations, unique, continuous, differentiable, fast to compute, and exhibits excellent empirical performance on benchmark datasets.