Many-Body Tensor Representation for Machine Learning of Solids

Haoyan Huo[1], Matthias Scheffler,[2] Matthias Rupp[2]

[1]School of Physics, Peking University, Beijing, China
[2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Accurate simulations of materials require electronic structure calculations whose high computational cost is a limiting factor. In high-throughput settings, machine learning can significantly reduce overall costs by interpolating between reference calculations. This approach requires a numerical representation of materials that supports interpolation. We present a many-body tensor representation that can encode both finite (molecules) and periodic systems (bulk crystal), has proper mathematical structure, is invariant to translation, rotation, and nuclear permutations, unique, continuous, differentiable, fast to compute, and exhibits competitive empirical performance on benchmark datasets. We demonstrate the approach for ab initio formation enthalpies of platinum-group / transition-metal binary alloys.