Message passing neural networks for partial charge assignment to metal-organic frameworks

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Virtual screenings can accelerate and reduce the cost of discovering metal-organic frameworks (MOFs) for their applications in gas storage, separation, and sensing. In molecular simulations of gas adsorption/diffusion in MOFs, the adsorbate-MOF electrostatic interaction is typically modeled by placing partial point charges on the atoms of the MOF. To virtually screen large libraries of MOFs, it is critical to develop computationally inexpensive methods to assign atomic partial charges to MOFs that accurately reproduce the electrostatic potential in their pores.

We design and train a message passing neural network (MPNN) to predict the atomic partial charges on MOFs under a charge neutral constraint. In an end-to-end manner, from crystal graphs representing MOFs, labeled with high-fidelity partial charges, our MPNN machine-learns features of the local bonding environments of the atoms and, from these features, learns to predict partial atomic charges. Our trained MPNN assigns high-fidelity partial point charges to MOFs with orders of magnitude lower computational cost (runtime: ~3 s) than electronic structure calculations.