Beyond Point Charges: Dynamic Polarization from
Neural Net Predicted Multipole Moments

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Abstract
Intramolecular polarization is the change to the electron density of a given atom upon variation in the positions of the neighbouring atoms. We express the electron density in terms of multipole moments. Using glycine and N-methylacetamide (NMA) as pilot systems, we show that neural networks can capture the change in electron density due to polarization. After training, modestly sized neural networks successfully predict the atomic multipole moments from the nuclear positions of all atoms in the molecule. Accurate electrostatic energies between two atoms can be then obtained via a multipole expansion, inclusive of polarization effects. As a result polarization is successfully modeled at short-range and without an explicit polarizability tensor. This approach puts charge transfer and multipolar polarization on a common footing. The polarization procedure is formulated within the context of Quantum Chemical Topology (QCT). Non-bonded atom-atom interactions in glycine cover an energy range of 948 kJmol⁻¹, with an average energy difference between true and predicted energy of 0.2 kJmol⁻¹, the largest difference being just under 1 kJmol⁻¹. Very similar energy differences are found for NMA, which spans a range of 281 kJmol⁻¹. The current proof-of-concept enables the construction of a new protein force field that incorporates electron density fragments that dynamically respond to their fluctuating environment.