Machine learned interatomic potentials for carbon and other elemental materials

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There is a long tradition in computational chemistry and materials science of representing the Born-Oppenheimer potential energy surfaces of materials using empirical force fields on the one hand, and also, for the most simple systems, systematic expansions of the potential energy function. Although the diverse range of potentials available for carbon, together with approximate quantum mechanical treatments, have enabled much understanding through molecular dynamics simulations of the diverse forms of carbon materials, it was widely felt that we have reached a plateaux in the attainable accuracy and therefore some phenomena were just out of reach. The formalism of "machine learning" (non-parametric function fitting in high dimensions) unites the previous two approaches. New kinds of parametrisations are the result, with a computational expense in between that of simple force fields and quantum chemistry. Recent work in my group include potentials for amorphous carbon, methane, and many other elemental materials, all of which significantly push the boundaries of accuracy.