Physics-based potentials across chemical space parametrized from machine learning

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Computer simulations are increasingly acquiring the necessary speed and accuracy to tackle rational materials design. The screening of many compounds requires transferable force fields, so as to alleviate tedious parametrization efforts for every new compound. In this talk, I will describe efforts aimed at optimizing classical intermolecular potentials that do away with a manual parametrization of every new molecule. By a combination of a machine-learning-based prediction of atomic properties, coupled with specific physics-based interactions, the model only includes 8 global parameters---optimized once and for all across compounds. The model is validated on gas-phase dimers, where chemical accuracy (1 kcal/mol) is reached for several datasets representative of non-covalent interactions in biologically-relevant molecules. We further focus on hydrogen-bond complexes---essential but challenging due to their directional nature---where datasets of DNA base pairs and amino acids yield an extremely encouraging 1.4 kcal/mol error.