Δ-Machine Learned Potential Energy Surfaces and Dynamics with Them

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There has been great progress in developing machine-learned potential energy sur- faces (PESs) for molecules and clusters with more than 10 atoms. Unfortunately, this number of atoms generally limits the level of electronic structure theory to less than the "gold standard" CCSD(T) level. Indeed, for the well-known MD17 dataset for molecules with 9-20 atoms, all of the energies and forces were obtained with DFT calculations (PBE). This talk is focused on a Δ-Machine Learning method we recently pro-posed and applied to bring DFT-based PESs to close to CCSD(T) accuracy. This is demonstrated for hydronium, N -methyl acetamide, acetyl acetone, and ethanol. For 15-atom tropolone it appears that special approaches, e.g., Molecular Tailoring, local CCSD(T), are needed to obtain the CCSD(T) energies. A new aspect of this approach is the extension of Δ-Machine Learning to force fields. The approach is based on many- body corrections to polarizable force fields potential. This is examined in detail using the TTM2.1 water potential. The corrections make use of our recent CCSD(T) datasets for 2-b, 3-b, and 4-b interactions for water. These datasets were used to develop a new fully *ab initio* potential for water, termed q-AQUA. Several dynamics calculations using the PES will be presented.