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Optimization of a van der Waals Density Functional for water[1]
MICHELLE FRITZ, Universidad Autonoma de Madrid, MARIVI FERNANDEZ-SERRA, Stony Brook University, JOSE M. SOLER, Universidad Autonoma de Madrid — In particularly delicate systems, like liquid water, ab initio exchange and correlation functionals are simply not accurate enough for many practical applications. In these cases, fitting the functional to reference data is a sensible alternative to empirical interatomic potentials. However, a global optimization requires functional forms that depend on many parameters and the usual trial and error strategy becomes cumbersome and suboptimal. We present a general and powerful optimization scheme called data projection onto parameter space (DPPS). In an arbitrarily large parameter space, DPPS expands the vector of unknown parameters in vectors of known data. Poorly sampled subspaces are determined by the physically-motivated functional shape of ab initio functionals, using Bayes' theory to combine this prior information with reference energies and electron densities of monomers, clusters, and condensed phases of water.

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