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A general optimization method applied to a vdW-DF functional for water MICHELLE FRITZ, JOSE M. SOLER, Universidad Autnoma de Madrid, MARIVI FERNANDEZ-SERRA, Stony Brook University — 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 have developed a general and powerful optimization scheme called data projection onto parameter space (DPPS) and applied it to the optimization of a van der Waals density functional (vdW-DF) for water. In an arbitrarily large parameter space, DPPS solves for vector of unknown parameters for a given set of known data, and poorly sampled subspaces are determined by the physically-motivated functional shape of ab initio functionals using Bayes' theory. We present a new GGA exchange functional that has been optimized with the DPPS method for 1-body, 2-body, and 3-body energies of water systems and results from testing the performance of the optimized functional when applied to the calculation of ice cohesion energies and ab initio liquid water simulations. We found that our optimized functional improves the description of both liquid water and ice when compared to other versions of GGA exchange.

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