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Optimization of van der Waals Density Functionals using Data Projection onto Parameter Space (DPPS) MICHELLE FRITZ, Universidad Autonoma de Madrid, MARIVI FERNANDEZ-SERRA, Stony Brook University, MIKE GILLAN, University College London, JOSE M. SOLER, Universidad Autonoma de Madrid — The parameterization and optimization of complex models fitted to reproduce a reference data set is an important part of the development of interatomic potentials. It is an approach that can also be used to design exchange and correlation functionals in density functional theory. Generally, this is a problem that requires choosing functional forms that depend on many parameters. The balance between the number of parameters and the size of the fitted data sets involves difficult and subjective decisions that are nevertheless critical for obtaining good results. We present a general and powerful optimization scheme, data projection onto parameter space (DPPS). The DPPS method tries to find the optimal parameters for a complex model which depends on a scalar function F which is determined by a large number of variables and parameters. The procedure involves the projection a vector of unknown parameters onto the vectors of known data. As an example, we apply DPPS to the optimization of the local exchange in a vdW density functional (vdW-DF). Our goal is to obtain an improved vdW-DF for water. To do so, we use an accurate potential energy surface for the water dimer as our initial data set.

Michelle Fritz
Universidad Autonoma de Madrid

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