A non-empirical improvement of PBE and its hybrid PBE0\textsuperscript{1} ALBERTO VELA, Departamento de Química, Cinvestav, JORGE M. DEL CAMPO, Departamento de Física y Química Teórica, UNAM, JOSE L. GAZQUEZ, Departamento de Química, UAM-Iztapalapa, S.B. TRICKEY, Quantum Theory Project, Physics & Chemistry, U. Florida — We present a non-empirical re-parameterization of the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) exchange-correlation functional and of the related PBE hybrid (PBE0) obtained by imposing the constraint that, for the hydrogen atom, the exchange energy cancels the Coulomb repulsion energy. The new parameterization is validated with well-known test sets. The results for the re-parameterized PBE GGA, called PBEmol, show a substantial improvement over the original PBE in predicted heats of formation, while retaining the quality of the original PBE functional for description of all the other properties considered. The results for the hybrids indicate that, although the PBE0 functional provides a rather good description of those properties, the predictions of the re-parameterized functional are, except in the case of the ionization potentials, modestly better. Also, the results are better than B3LYP, except for the case of the ionization potentials and the harmonic frequencies.

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