A non-empirical improvement of PBE and its hybrid PBE0[1] AL-
BERTO VELA, Departamento de Química, Cinvestav, JORGE M. DEL CAMPO,
Departamento de Física y Química Teórica, UNAM, JOSÉ L. GÁZQUEZ, Depar-
tamento 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 forma-
tion, 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 pre-
dictions 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.

Alberto Vela
Departamento de Química, Cinvestav

Date submitted: 09 Dec 2011   Electronic form version 1.4