ERRATA

Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]

John P. Perdew, Kieron Burke, and Matthias Ernzerhof

[S0031-9007(97)02302-8]

For the molecules Be_2, F_2, and P_2 of Table I, the unrestricted Hartree-Fock solution breaks the singlet spin symmetry, even though the density-functional solutions do not. For these broken-symmetry solutions, the UHF atomization energies become $+7$, -20, and $+41$ kcal/mol, respectively, and the mean absolute error of all the UHF atomization energies becomes 69.8 kcal/mol.

The PBE correlation energy of the two-electron ions of nuclear charge $Z \rightarrow \infty$ should be corrected to -0.0479 hartree, consistent with the PBE value $\omega = 0.046644$ stated in the Letter. The quoted value -0.0482 hartree was obtained from the more refined $\omega = 0.046920$ of G. G. Hoffman, Phys. Rev. B **45**, 8730 (1992).

Reference [6] should have been "A. C. Scheiner, J. Baker, and J. W. Andzelm, J. Comput. Chem. (to be published)".

 0031-9007/97/78(7)/1396(1)$10.00