JCTC Journal of Chemical Theory and Computation

Erratum

pubs.acs.org/JCTC

Correction to Construction of the B88 Exchange-Energy Functional in Two Dimensions

J. G. Vilhena,* E. Räsänen,* M. A. L. Marques, and S. Pittalis

J. Chem. Theory Comput. **2014**, *10* (5), 1837−1842. DOI:10.1021/ct4010728

Below eq 14, we wrote: "*Using eq 14 in eqs 3 and 11, we find that the LDA exchange energies are on the order of* $N^{4/3}$*,...*". Instead, since we are discussing the two-dimensional (2D) case (not the three-dimensional one), we should have written: "*Using eq 14 in eqs 8 and 11, we find that the LDA exchange energies are on the order of* $N^{3/2}$*,...*". Therefore, Figure 3 should be replaced with Figure 1 reported here.

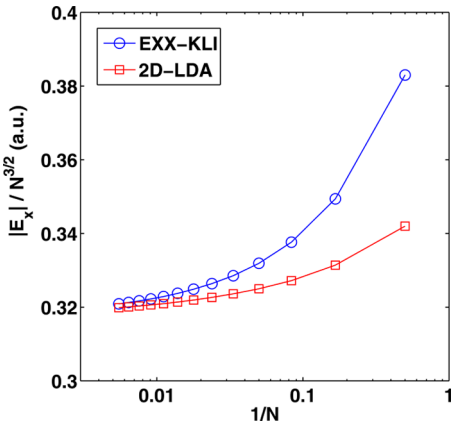

Figure 1. Comparison of exchange energies of the exact-exchange scheme in the KLI approximation and of the 2D local-density approximation (2D-LDA) for a set of 2D parabolic quantum dots on the order of $N^{3/2}$ (see text). The KLI results approach the LDA values for increasing N. The number of electrons and confinement potentials of the systems are scaled according to eq 13.

We thank Gabriel José Gil Pérez for pointing out these mistakes to us. They do not affect the main results but create confusion in the analysis that illustrates our procedure. This erratum resolves the issue.

Published: September 22, 2015

DOI: 10.1021/acs.jctc.5b00860
J. Chem. Theory Comput. 2015, 11, 5054−5054