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Correction: Localization in the SCAN meta-generalized gradient approximation functional leading to broken symmetry ground states for graphene and benzene

Yubo Zhang,^{ab} Wenqing Zhang^{*ab} and David J. Singh^{*cd}

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Correction for 'Localization in the SCAN meta-generalized gradient approximation functional leading to broken symmetry ground states for graphene and benzene' by Yubo Zhang *et al.*, *Phys. Chem. Chem. Phys.*, 2020, 22, 19585–19591, DOI: 10.1039/D0CP03567J.

The energy for the experimental curve in Fig. 1a of the paper was plotted per molecule rather than per atom. The correct curve is above the LDA and closer to PBE. Accordingly, the phrase “The LDA shows accord with experiment as far as the binding energy and bond length is concerned” should be changed to “The LDA shows accord with experiment as far as the bond length is concerned” and “The PBE also shows a reasonable accord with experiment in terms of the bond length, but it has an under-binding in terms of energy” should be changed to “The PBE shows a reasonable accord with experiment in terms of bond length and energy”. The calculated results and the conclusions regarding the SCAN functional are unchanged. We thank John Perdew for pointing this out and apologize for the inconvenience caused by this error.

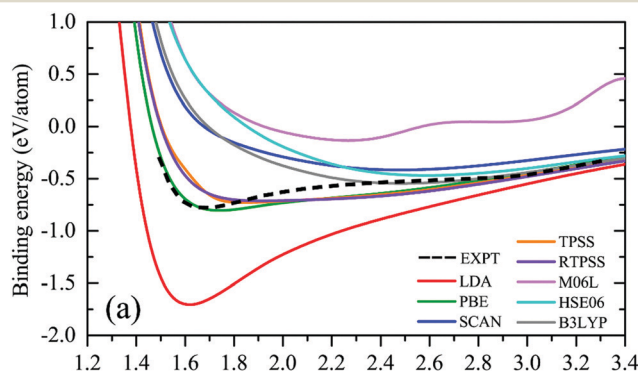


Fig. 1 (a) Binding energy curves for the neutral Cr dimer using different density functionals.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

^a Department of Physics and Shenzhen Institute for Quantum Science & Engineering, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China. E-mail: zhangwq@sustech.edu.cn

^b Guangdong Provincial Key Lab for Computational Science and Materials Design, and Shenzhen Municipal Key Lab for Advanced Quantum Materials and Devices, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China

^c Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, USA. E-mail: singhdj@missouri.edu

^d Department of Chemistry, University of Missouri, Columbia, MO 65211, USA

