Main-group test set for materials science and engineering with user-friendly graphical tools for error analysis: systematic benchmark ofthe numerical and intrinsic errors in state-of-the-art electronic-structure approximations

Igor Ying Zhang[1,2], Andrew J Logsdail[3], Xinguo Ren[4], Sergey V Levchenko[1,5], Luca Ghiringhelli[1], and Matthias Scheffler[1]

[1] Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany
[2] Department of Chemistry, Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, and MOE Key Laboratory of Computational Physical Science, Fudan University, Shanghai 200433, People s Republic of China
[3] Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, United Kingdom
[4] CAS Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei 230026, People s Republic of China
[5] Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, 3 Nobel Street, 143026 Moscow Russia; National University of Science and Technology 'MISIS', 119049 Moscow, Russia

Understanding the applicability and limitations of electronic-structure methods needs careful and efficient comparison with accurate reference data. Knowledge of the quality and errors of electronic-structure calculations is crucial to advanced method development, high-throughput computations and data analyses. In this paper, we present a main-group test set for computational materials science and engineering (MSE) [1], that provides accurate and easily accessible crystal properties for a hierarchy of exchange-correlation approximations, ranging from the well-established mean-field approximations to the state-of-the-art methods of many-body perturbation theory. We consider cohesive energy, lattice constant and bulk modulus of a set of materials that representatives for the first- and second-row elements and their binaries with cubic crystal structures and various bonding characters. A strong effort is made to achieve high numerical accuracy for cohesive properties as calculated using the local-density approximation (LDA), several generalized gradient approximations (GGAs), meta-GGAs

and hybrids in all-electron resolution, and the second-order Møller–Plesset perturbation theory (MP2) and the random-phase approximation (RPA) both with frozen-core approximation based on all-electron Hartree–Fock, PBE and/or PBE0 references [2, 3]. This results in over 10 000 calculations, which record a comprehensive convergence test with respect to numerical parameters for a wide range of electronic-structure methods within the numerical atom-centered orbital framework. As an indispensable part of the MSE test set, a web site is established http://mse.fhi-berlin.mpg.de. This not only allows for easy access to all reference data but also provides user-friendly graphical tools for post-processing error analysis.

References

[1] I. Y. Zhang *et al.* New J. Phys. **21**, 013025 (2019).

[2] I. Y. Zhang, X. Ren, P. Rinke, V. Blum, and M. Scheffler, New J. Phys. **15**, 123033 (2013).

[3] X. Ren, P. Rinke, C. Joas, and M. Scheffler, J. Mater. Sci. **47**, 7447 (2012).