

Abstract Submitted
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Test of a nonempirical density functional for short-range van der Waals interaction in rare-gas dimers¹ JIANMIN TAO, JOHN PERDEW, Department of Physics, Tulane University, New Orleans, LA 70118 — It is known that the nonempirical generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) provides a much more realistic description of the short-range part of the van der Waals (vdW) interaction than does the local spin density (LSD) approximation. In the present work, the ability of the higher-level nonempirical meta-GGA of Tao, Perdew, Staroverov, and Scuseria (TPSS) [Phys. Rev. Lett. **91**, 146401 (2003)] to describe vdW interaction is tested self-consistently in rare-gas dimers with $Z \leq 36$. The one-parameter hybrid version (TPSSh) of the TPSS exchange-correlation functional is also included in this test. Calculations show that both TPSS and TPSSh functionals correctly yield vdW bonds in these dimers and significantly improve the prediction of bond lengths and binding energies over LSD. The rather close agreement of TPSS with PBE for these dimers confirms a principle of the TPSS construction: preservation of the PBE large-gradient behavior. Compared with the PBE GGA, TPSS and TPSSh yield a slightly weaker binding. The typically too-long bond lengths and too-small binding energies of TPSS meta-GGA suggest the need for some long-range vdW interaction correction which is discussed.

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