Long-Range van der Waals Correction to a Semilocal Density Functional: The Tail Need Not Wag the Dog[1]

JOHN P. PERDEW, Temple University

The SCAN [1] (strongly constrained and appropriately normed) meta-generalized gradient approximation satisfies all 17 exact constraints that a semilocal functional can. Without being fitted to any bonded system, it correctly describes most kinds of bonding [2], including intermediate-range van der Waals (vdW) interaction. It can be supplemented [3.4] with a long-range vdW correction such as D3 or rVV10, which have the flexibility to exclude any intermediate-range contribution. Accurate results are found for free molecules [3], for molecules weakly bound to metal surfaces [4], and for interlayer binding energies of layered materials [4]. Despite being a pair-interaction model, the rVV10 correction to SCAN also gives a random-phase-approximation-like long-range contribution to the binding energy curve for graphene on a nickel surface [4]. [1] J. Sun, A. Ruzsinszky, and J.P. Perdew, Phys. Rev. Lett. **115**, 036402 (2015). [2] J. Sun *et al.*, Nature Chem. **8**, 831 (2016). [3[J.G. Brandenburg, J.E. Bates, J. Sun, and J.P. Perdew, Phys. Rev. B **94,** 115144 (2016). [4] H. Peng, Z. Yang, J.P. Perdew, and J. Sun, Phys. Rev. X **6**, 041005 (2016).