A Higher-Accuracy van der Waals Density Functional

Kyuho Lee,[1] Éamonn D. Murray,[1] Lingzhu Kong,[1] Bengt I. Lundqvist,[2,3] and David C. Langreth[1]

[1]*Department of Physics and Astronomy, Rutgers University Piscataway, NJ, USA*

[2]*Department of Applied Physics, Chalmers University of Technology SE - 41296 Göteborg, Sweden*

[3]*Center for Atomic-scale Materials Design, Department of Physics Technical University of Denmark, DK - 2800 Kongens Lyngby, Denmark*

We propose[1] a second version of the van der Waals density functional (vdW-DF2) of Dion et al.,[2] employing a more accurate semilocal exchange functional and the use of a large-N asymptote gradient correction in determining the vdW kernel. We show that equilibrium separations, hydrogen bond strengths, and van der Waals attractions at intermediate separations longer than equilibria are greatly improved in this second version vdW-DF2.

[1] Kyuho Lee, Éamonn D. Murray, Lingzhu Kong, Bengt I. Lundqvist, and David C. Langreth, arXiv:1003.5255v1 (2010).

[2] M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, and B. I. Lundqvist, Phys. Rev. Lett. **92**, 246401 (2004).