van der Waals Coefficients for Nanostructures: Fullerenes Defy Conventional Wisdom

Adrienn Ruzsinszky[1], John P. Perdew[1], Jianmin Tao[1], Gábor I. Csonka[2], and J.M. Pitarke[3,4]

[1] Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118

[2] Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, H-1521 Budapest, Hungary

[3] CIC nanoGUNE Consolider, E-20018 Donostia-San Sebastian, Basque Country, Spain

[4] Materia Kondentsatuaren Fisika Saila, DIPC, and Centro Fisica Materiales CSIC-UPV/EHU, 644 Posta Kutxatila, E-48080 Bilbo, Basque Country, Spain

Weak van der Waals interactions are responsible for many useful mechanical features of nanostructures. Fullerene molecules such as C_{60} are large nearly-spherical shells of carbon atoms. The van der Waals coefficients between quasispherical nanostructures can be modeled accurately and analytically by those of classical solid spheres (for nanoclusters) or spherical shells (for fullerenes) of uniform valence electron density, with the true static dipole polarizability. Here I will derive analytically and confirm numerically from this model the size-dependences of the van der Waals coefficients of all orders, showing for example that the asymptotic dependence for C_6 is the expected n^2 for pairs of nanoclusters A_n-A_n, each containing n atoms, but $n^{2.75}$ for pairs of single-walled fullerenes C_n-C_n. Large fullerenes are argued to have much larger polarizabilities and dispersion coefficients than those predicted by either the standard atom pair-potential model or widely-used nonlocal van der Waals correlation energy functionals. The failure of these nonlocal van der Waals functionals is known for metallic systems but is less known for hollow systems such as fullerenes or nanostructures with a cavity.

Ruzsinszky, A., Perdew, J.P., Tao, J., Csonka, G.I, and Pitarke, J.M. Phys. Rev. Lett.**109**, 233203, (2012).

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

O.A. Vydrov and T. Van Voorhis, Phys. Rev. A **81**, 062708 (2010).

J. Tao, J.P. Perdew, and A. Ruzsinszky, Phys. Rev. B **81**, 233102 (2010).

J. Tao, J.P. Perdew, and A. Ruzsinszky Proc. Nat. Acad. Sci. (USA) **109**, 18 (2012).

J.P. Perdew, J. Tao, P. Hao, A. Ruzsinszky, G.I. Csonka, and J.M. Pitarke, J. Phys.: Condens. Matter **24**, 424207 (2012).

A.A. Lucas, L. Henrard, and Ph. Lambin, Phys. Rev. B **49**, 2888 (1994).

J.F. Dobson, A. White, and A. Rubio, Phys. Rev. Lett. **96**, 073201 (2006).

A. Tkatchenko, R.A. DiStasio, R. Car, and M. Scheffler, Phys. Rev. Lett. **108**, 236402 (2012).