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Abstract for an Invited Paper
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Modern theory of van der Waals interactions[1]

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van der Waals (vdW, dispersion) interactions [1,2,3] are important in diverse areas such as colloid, surface and nano science, cohesion of molecular crystals, and biomolecular science. They also provide competition in experiments to discover the fifth fundamental force.While vdW interactions have been understood in principle for a century, their quantitative first-principles prediction and modelling down to chemical contact separations have proven stubbornly difficult because the quantal many-electron problem is involved. After some brief historical material, the current state of the art will be discussed with particular reference to several approaches: pairwise additive [4,5,6], perturbative [7,8] quantum chemical [9], vdW-DF [10,11], Lifshitz-like scattering[1,2,12], RPA-like [13-17], Adiabatic Connection Fluctuation Dissipation / Time Dependent DFT based [18,19] etc.. A potentially useful classification will be introduced to aid in understanding the physical causes of departures from pairwise additivity, that is from the usual sum of C_6R^{-6} contributions. These departures result in non-standard power law decays of nanostructure vdW interactions as a function of separation D [13], as well as surprising dependences of the attraction on the number, N, of atoms within each vdW-interacting fragment [20,21]. Some further recent results on non-additivity will also be presented [22]. REFERENCES. [1] V. A. Parsegian, "van der Waals Forces," Cambridge University Press, Cambridge 2005: [2] J. F. Dobson and T. Gould, J. Phys. Condens. Matter 24, 073201 (2012): [3] J. Klimes & A. Michaelides, J. Chem. Phys. 137, 120901 (2012) : [4] S. Grimme, J. Antony, S. Ehrlich, et al., J. Chem. Phys. 132, 154104 (2010): [5] S. Ehrlich, J. Moellmann, and S. Grimme, Acc. Chem. Research 46, 916 (2013): [6] R. Sedlak, T. Janowski, M. Pitonak et al., J. Chem. Th. Comput. 9, 3364 (2013): [7] B. Jeziorski, R. Moszynski, and K. Szalewicz, Chem. Rev. 94, 1887 (1994): [8] D. Kuchenbecker and G. Jansen, Chem. Phys. Chem. 13, 2769 (2012): [9] J. Rezac, L. Simova, and P. Hobza, J. Chem. Th. Comput. 9, 364 (2013): [10] M. Dion, H. Rydberg, E. Schroder, et al., Phys. Rev. Lett. 92, 246401 (2004): [11] K. Berland and P. Hyldgaard, Phys Rev B 87, 205421 (2013): [12] S. J. Rahi, T. Emig, N. Graham, et al., Phys. Rev. D 80, 085021 (2009): [13] J. F. Dobson, A. White and A. Rubio, Phys. Rev. Lett. 96, 073201 (2006): [14] S. Lebegue, J. Harl, T. Gould, et al., Phys. Rev. Lett. 105, 196401 (2010): [15] A. Tkatchenko, R. di Stasio, R. Car, et al., Phys. Rev. Lett. 108, 236402 (2012): [16] T. Bucko, S. Lebegue, J. Hafner, J. G. Angyan, Phys. Rev. B. 87, 064110 (2013): [17] A. Gruneis, J. Harl, M. Marsman, et al., J. Chem. Phys. 131, 154115 (2009): [18] T. Gould, J. Chem. Phys. 137, 111101 (2012): [19] T. Olsen and K. Thygesen, Phys. Rev. B 88, 115131 (2013): [20] A. Ruzsinszky, J. P. Perdew, J. Tao et al., Phys. Rev. Lett. 109, 233203 (2012): [21] V. V. Gobre and A. Tkatchenko, Nature Comm. 4, 2341 (2013): [22] J. F. Dobson, A. Savin, J.A. Angyan, and R.F. Liu, unpublished.

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