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**Towards Efficient and General Method for Many-Body van-der-Waals Interactions** ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin — Van der Waals interactions are intrinsically many-body phenomena, arising from collective electron fluctuations in a given material. Adiabatic connection fluctuation-dissipation theorem (ACFDT) allows to compute the many-body vdW interactions accurately. However, the ACFDT computational cost is prohibitive for real materials, even when the random-phase approximation is employed for the response function. We show how the problem of computing the long-range many-body vdW energy for real systems can be solved efficiently by mapping the system (molecule or condensed matter) onto a collection of quantum harmonic oscillators. Currently, our method, which couples density-functional theory with the many-body dispersion energy (DFT+MBD), is developed for non-metallic system [A. Tkatchenko, R. A. DiStasio Jr., R. Car, M. Scheffler, submitted]. The DFT+MBD method includes the hybridization effects by using the Tkatchenko-Scheffler approach [PRL 102, 073005 (2009)], the long-range Coulomb screening through classical electrodynamics [B. U. Felderhof, Physica 29, 1569 (1974)], and the many-body vdW energy from the coupled-fluctuating dipole model [M. W. Cole et al., Mol. Simul. 35, 849 (2009)]. The successes of the DFT+MBD approach and the many challenges that lie ahead will be discussed.

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