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Extending the applicability of Many-Body Dispersion (MBD) to large-scale systems: DFTB+MBD MARTIN STÖHR, Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg, REINHARD J. MAURER, Department of Chemistry, Yale University, New Haven, CT 06520, USA, ALEXANDRE TKATCHENKO, Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — The inclusion of van der Waals (vdW) dispersion interactions in electronic-structure calculations has significantly extended the applicability of DFT. However, the accessible system sizes with DFT+vdW remain small for many practically relevant applications. On the other hand, Density-Functional Tight-Binding (DFTB) is an electronic-structure method of choice for systems with several 1000s of atoms. A severe drawback of DFTB and other semi-empirical methods, however, is the missing direct access to atomic polarizabilities, required for most common *ab initio* vdW models. Here, we present a novel approach to derive accurate effective polarizabilities directly from the atom-centered basis set representation of the density-matrix [1]. This enables the use of sophisticated dispersion models such as the Many-Body Dispersion (MBD) scheme [2] in conjunction with most electronic-structure methods including both DFT and DFTB, thus allowing the investigation of many-body effects in large-scale systems. We exemplify the viability of such a combined approach by adressing the impact of many-body dispersion on the solvation effect in biomolecular systems with DFTB+MBD. [1] M. Stöhr et al., J. Chem. Phys. 144, 151101, 2016; [2] A. Tkatchenko et al., Phys. Rev. Lett. 108, 236402, 2012.

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