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Efficient Oscillator-Based Approach for Polarizability and van der Waals Interactions VIVEKANAND GOBRE, Fritz-Haber-Institut der MPG, ROBERT A. DISTASIO, JR., ROBERTO CAR, Princeton University, USA, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG — The dynamic polarizability measures the response to an applied time-dependent electric field, and its accurate determination is crucial for van der Waals (vdW) interactions and other response properties. First-principles calculations of polarizabilities in principle require a computationally expensive explicit treatment of many-electron excitations, and are only applicable in practice to systems with less than about 100 atoms. In this work, we present an efficient parameter-free approach for calculating accurate frequency dependent polarizabilities for molecules with thousands of atoms, as well as periodic materials. This is achieved by the synergistic coupling of the Tkatchenko-Scheffler method [1], which accurately treats short-range hybridization effects, with the self-consistent screening equation from classical electrodynamics [2,3]. Using only the electron density and free atom reference, we obtain an accuracy of 7% for both static polarizabilities and vdW coefficients for an extensive database of gas-phase molecules and crystals. We analyze the interplay of hybridization and long-range electrostatic screening effects on the polarizability. [1] Tkatchenko and Scheffler, PRL (2009), [2] Felderhof, Physica (1974), [3] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012).

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