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The Role of Many-Body Dispersion Interactions in Molecular Crystals

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The structure, energetics, and electronic properties of molecular crystals are studied using density functional theory (DFT) with the recently developed many-body dispersion (MBD) method [Tkatchenko et al. Phys. Rev. Lett. 108, 236402 (2012)]. It is shown that accounting for the long-range electrostatic screening in extended systems is essential for obtaining the correct dielectric constants and ensuing optical properties of molecular crystals [Schatschneider et al., arXiv:1211.1683]. Furthermore, accounting for the non-additive many-center dispersion interactions is crucial for obtaining a highly accurate description of the energetics of molecular crystals. This includes lattice energies, sublimation enthalpies [Reilly et al., to be published], and relative stabilities of polymorphs [Marom et al. arXiv: 1210.5636]

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