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Towards Reliable Predictions of Molecular Materials ANTHONY REILLY, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG, Berlin, Germany — While dispersion interactions are known to be essential to the stability and accurate prediction of molecular-crystal structures, the vast majority of computational methods use simple pairwise approximations to model these interactions, ignoring the non-additive, many-body nature of long-range electron correlation. Here we use the recently developed many-body dispersion (MBD) method (PRL 108, 236402; PNAS 109, 14791) together with a representative database of molecular crystals, to illustrate how important electrodynamic screening and many-body contributions are to crystal stability. Crucially, these MBD contributions allow DFT calculations to reach the highly coveted “chemical accuracy” with respect to high-level calculations and experiments in both the crystalline and gaseous phases. This ability to treat molecular solids and their components on such an accurate and equal footing is essential for controlled and informed design of complex materials.

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