

# Oral Contributions

**[MS23-05] Reliable Modelling of Stability and Polymorphism of Molecular Crystals with Many-Body van der Waals Interactions.**  
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Density-functional theory (DFT) based methods are increasingly being used to study the structure and polymorphism of molecular crystals.[1] The crucial importance of van der Waals (vdW) interactions in such studies is now widely accepted. However, many vdW-inclusive DFT approaches, as well as force fields, employ pairwise models for dispersion interactions, [2] neglecting the true non-additive many-body nature of these effects.[3] In this contribution we show how many-body vdW contributions can be essential for correctly modelling the energetics of molecular crystals. We introduce a database of 23 molecular crystals, for which accurate values of experimental lattice energies have been determined using experimental sublimation enthalpies.[4, 5] Comparison of DFT lattice energies with the experimental values shows that only the recently developed many-body dispersion (MBD) method[6,7] is capable of reaching the coveted “chemical accuracy” benchmark, achieving a mean absolute error of 3.9 kJ/mol when coupled with the PBE0 hybrid functional. The importance of many-body contributions for polymorphism is highlighted using the examples of glycine, oxalic acid and aspirin.[4, 8] In particular, many common pairwise methods and force fields fail to predict the correct polymorphic stability of glycine and oxalic acid, while the MBD approach correctly reproduces the experimentally known ordering of these systems.[8] Overall, the results presented show that the approach outlined here is capable of meeting the challenging demands of crystal-structure prediction and organic material design with minimal empiricism.

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