Contribution ID : **44** Type : **Oral Presentation**

Multi-level coupled-cluster description of crystal lattice energies

The many-body expansion (MBE) of the lattice energy offers a route to an ab initio description of molecular solids based on systematic wave-function approximations. However, MBE can only be practical if one can deal with the daunting number of n-body contributions. To this end, we employ a multi-level approach (Figure 1). CCSD(T) is only required for the first and second coordination shells. At longer distances and for the three-body interactions, RPA with third-order corrections [1] is sufficient. The extremely long-range and beyond three-body interactions appear to be driven by the mean field and can be efficiently accounted for at the Hartree-Fock level with periodic boundary conditions.

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