MnO₂ Polymorph Energetics – A Unique Theoretical Challenge

Scientific Achievement

Through a collaboration with the CCDM EFRC, we have established that the new, non-empirical, SCAN* exchange-correlation functional for density functional theory provides a uniquely accurate first-principles model of polymorph energetics and properties.

*Strongly Constrained and Appropriately Normed Semilocal Density Functional Sun et al., Phys Rev Lett 115, 036402 (2015).

Significance and Impact

Reliable and accurate first-principles approaches to access polymorph thermodynamics are key to understanding both the formation of metastable structures and the mechanisms of their synthesis.

Research Details

- Correctly identified polymorphs of MnO₂ (Fig. 1)
- Compared conventional methods to SCAN functional (Fig. 2)
- Identified physics underlying improvement with SCAN
- Calculated energetics and key properties (electronic, magnetic, and crystallographic structure) from first principles
- Identified domain of reliable applicability

Kitchaev et al., Phys Rev B 93, 045132 (2016).

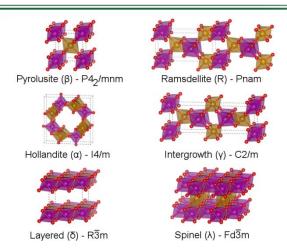


Fig. 1: Common polymorphs of MnO₂

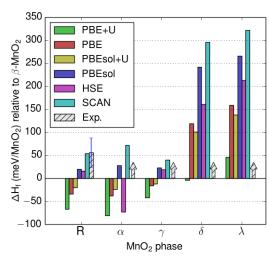


Fig. 2: Computed and experimental formation energies of MnO₂ polymorphs

















