MnO_2 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 **C**onstrained and **A**ppropriately **N**ormed 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 MnO_2 (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).

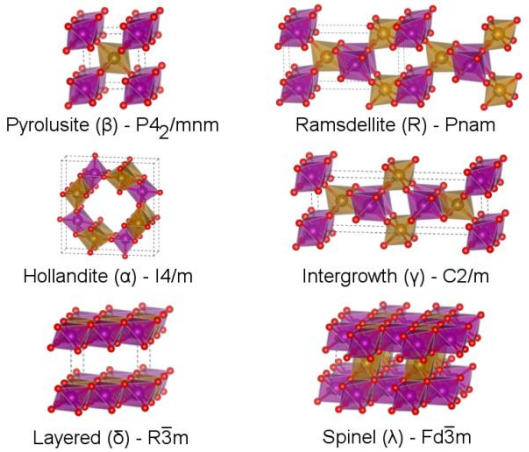

Fig. 1: Common polymorphs of MnO_2

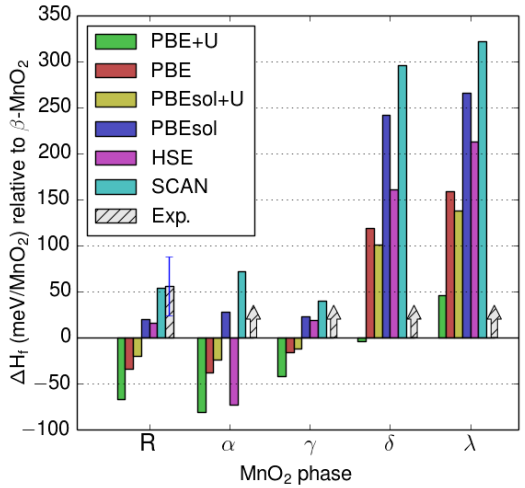

Fig. 2: Computed and experimental formation energies of MnO_2 polymorphs