Striking many-body effects in a simple oxide: the B2O3 case

Guillaume Ferlat*[1], Maria Hellgren , and Michele Casula

[1]Université Pierre et Marie Curie - Paris 6 (UPMC) – Institut de minéralogie, de physique des matériaux et de cosmochimie – 4 place Jussieu - 75005 Paris, France

Résumé

Boron oxide is a prototypical network-forming system made of trigonal units [1-4]. Of particular relevance is the existence of some specific units, called boroxol rings, which are the analogue of benzene rings in these oxides [1]. Here, we will show the striking effects of many-body, mostly van der Waals, contributions to the energy and structure of these materials using ab initio methods, including DFT at different levels up to RPA and QMC calculations [2]. This was achieved on a set of polymorphic crystalline structures which were predicted a few years ago [3]. The results, not only enrich the B2O3 phase diagram and explain anomalies of the glassy phase, but could also be used for the benchmarking of ab initio methods and for the calibration of new force-fields [4].

G. Ferlat *et al.*, Phys. Rev. Letters, **101** 065504 (2008).

G. Ferlat, M. Hellgren, F.-X. Coudert, H. Hay, F. Mauri and M. Casula, Phys. Rev. Mat., **3**, 063603 (2019).

G. Ferlat *et al.*, Nature Mater. **11**, 925 (2012).

A. Baroni *et al.*, J. Chem. Phys. **151**, 224508 (2019).

Mots-Clés: polymorphism, oxide, DFT, RPA, QMC

*Intervenant