Predicting new B_2O_3 polymorphs and their properties by ab initio calculations

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Despite its chemical simplicity, boron trioxide appears a puzzling system, as it does not crystallizes under normal conditions of temperature and pressure. It was hypothesized, based on DFT calculation in the GGA approximation, that this 'crystallization anomaly' resulted from the existence of a 'hidden' low energy polymorphism [1].
In a previous work, we showed that including dispersion effects was critical for an accurate description of the volume and energetics of SiO_2 polymorphs [2]. SiO_2 and B_2O_3 being the two textbook examples of network forming oxides, it is to be expected that dispersion effects also play a crucial role in the ab initio description of B_2O_3's hidden polymorphism. We consequently use van der Waals corrected density functional theory and Quantum Monte Carlo to investigate B_2O_3 polymorphs. We refined the predictions of Ref.[1], and we used this methodology to predict the properties of the newly found polymorphs. It is demonstrated that most structures have interesting mechanical properties, including high porosity, strong anisotropy, and negative linear compressibility.

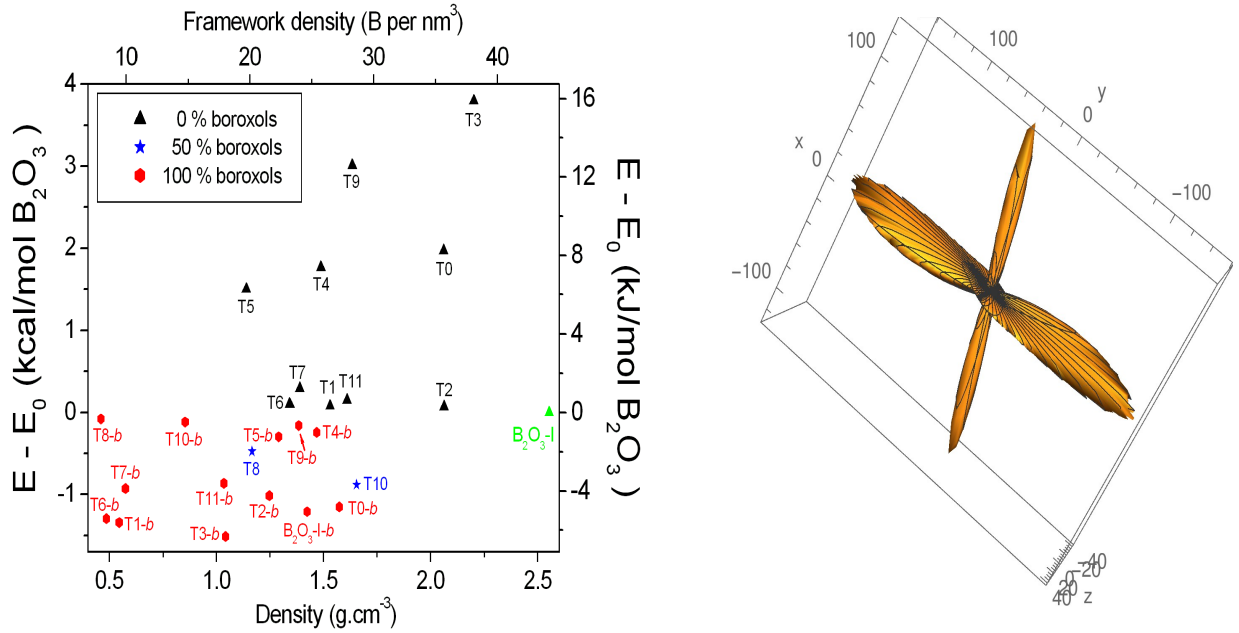

Figure 1. Left-Energy versus density plot showing predictions of a low energy polymorphism in B_2O_3 [1]. Right – Spatial dependence of the Young's modulus of one of the new polymorph show extreme anisotropy, with two orders of magnitude between the softest direction and the hardest.

Bibliography

[1] Guillaume Ferlat, Ari Paavo Seitsonen, Michele Lazzeri & Francesco Mauri, 'Hidden polymorphs drive vitrification in B_2O_3', *Nature Materials*, **11**, 925–929 **(2012)**.
[2] Henri Hay, Guillaume Ferlat, Michele Casula, Ari Paavo Seitsonen, and Francesco Mauri, 'Dispersion effects in SiO_2 polymorphs: An ab initio study', Phys. Rev. B, **92**, 144111, **(2015).**