Hidden polymorphism in B_2O_3 revealed from *ab initio* searches

Guillaume Ferlat[1], Henri Hay[1], Michele Casula[1], Ari P. Seitsonen[2], François-Xavier Coudert[3], Michele Lazzeri[1], Francesco Mauri[1],
[1]*Institut de Minéralogie, Physique des Matériaux et Cosmochimie (IMPMC), Université P. & M. Curie (UPMC), Paris, 75005, France;*[2]*Département de Chimie, ENS Paris, 75005, France;*
[3]*Chimie-ParisTech, 75005, Paris, France*.
E-mail: ferlat@impmc.upmc.fr

Using topological arguments (decoration of known networks) and *ab initio* energy calculations, we recently predicted the existence of 25 new B_2O_3 polymorphs (in addition to the known low-pressure B_2O_3-I phase) [1]. Interestingly, all these predictions have a low energy (typically comparable to the known phase) and a low density (for some of them comparable to silica zeolites). Being made of light elements and showing channel- or cage-like structures, these crystals may be promising for *e.g.* gas-storage applications. More fundamentally, we show that the existence of these polymorphs provide strong clues to understand the anomalous properties of the glassy phase (low density, presence of superstructural units known as boroxol rings, ease of vitrification and crystallization anomaly). The obtained polymorphism in B_2O_3 will be put in perspective with that of SiO_2, another network-forming system. We argue that the B_2O_3 polymorphism has so far remained *hidden* by the vitrification. Current directions to synthesize experimentally these phases will be discussed [2].

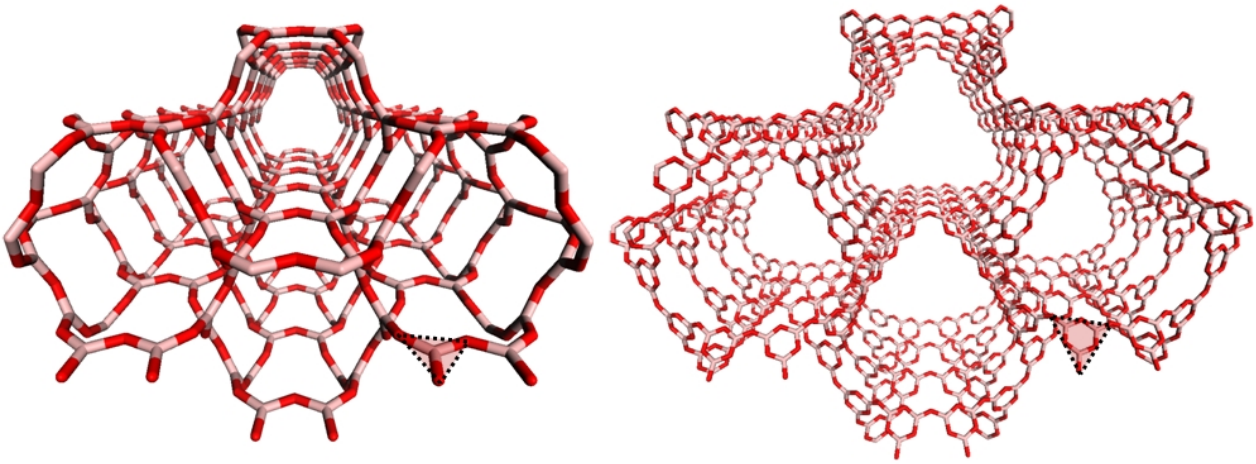

Figure 1. Two examples of B_2O_3 polymorphs among the 25 predictions of Ref. [1].

Bibliography

[1] G. Ferlat, A.P. Seitsonen, M. Lazzeri, F. Mauri, *Nature Materials*, **13**, 925 **(2012)**
[2] M. Daub, H. Hillebrecht, *Eur. J. Inorg. Chem.*, **2015**, 4176 **(2015)**