# Internship offered in M2
## 2018-2019

### Responsible for internship


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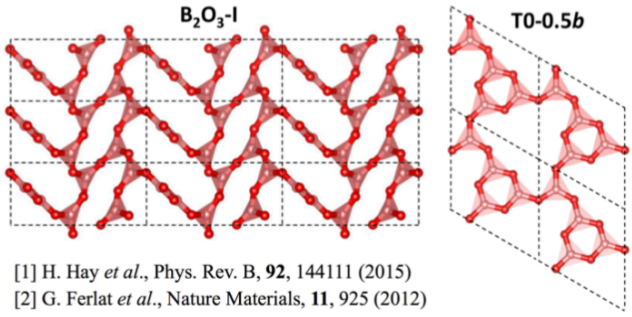
### Internship topic: *van der Waals interactions in glass-forming boron oxide*

van der Waals (vdW) interactions arise between neutral atoms from temporary dipoles caused by correlated electronic fluctuations. This weak attractive force is responsible for the structure and stability of many materials. A surprising and quite new discovery is the importance of the vdW interactions in glass forming compounds such as silica and boron oxide [1]. Boron oxide ($B_2O_3$) is one of the best glass formers but exhibit many unusual features. For example, there is a structural difference between its glassy (v-$B_2O_3$) and crystalline forms ($B_2O_3$-I). In v-$B_2O_3$, the elemental bricks are arranged into three-fold rings, referred to as boroxol rings, not present in $B_2O_3$-I. The formation of such rings stabilizes the glass structure for reasons which remain unclear. In Ref. [2] several new polymorphs with ring structures were found, and more recently we found that the vdW interactions change the energy landscape generating additional meta-stable structures within the same topology. The aim of this project is to gain a more detailed understanding of the interactions that are involved between the elemental bricks of the crystal, trying to explain why some structures are energetically favorable. We will also study how well different approximations in density functional theory perform by comparing to advanced many body methods.





[1] H. Hay *et al.*, Phys. Rev. B, **92**, 144111 (2015)
[2] G. Ferlat *et al.*, Nature Materials, **11**, 925 (2012)


Techniques involved: electronic structure codes: DFT and RPA
Applicant skills: strong background in solid-state/chemical physics, propensity for simulation and/or programming

Paid internship: Yes
Can this internship be continued for a PhD? Yes
If yes, type of PhD funding envisaged is: Ministère