

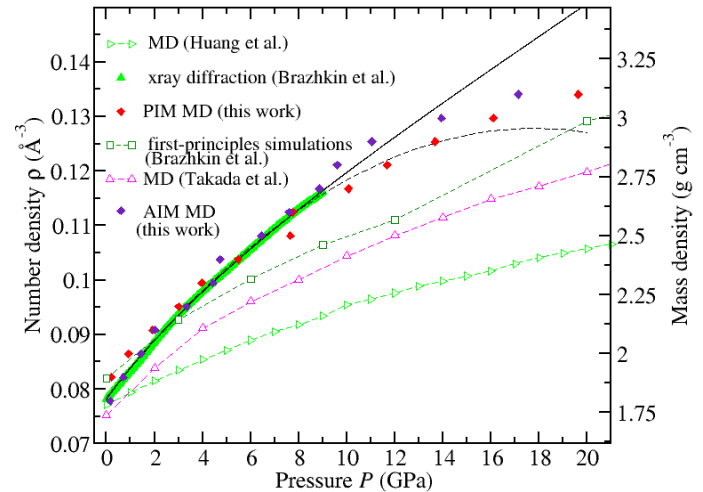
# Labex MATISSE

## Axe 5

« Project title » Toward a phase diagram of B2O3 pressure-temperature-concentration

Name Baroni Axelle

Hosting laboratories LPTMC, IMPMC ,PHENIX



Hosting laboratories, teams and and thesis supervisors names:

LPTMC :team Simulations moléculaires et modélisation des liquides, des verres et des géomatériaux ,thesis supervisor Matthieu Micoulaut

We study structural transformations of boron trioxyde under high pressure and high temperature thanks to molecular dynamic simulations including polarisable potentials fitted from ab-initio simulations. Several potentials have been obtained and tested on boron trioxyde in 3 phases : liquid, glassy and cristaline. We have studied the evolution of basic structural units under temperature and pressure in order to understand how these basic structural units were transformed under these parameters, whatkind of new structural units were obtained and in what way they are responsible for transport properties.

Summarize your scientific results & impacts (5 lines)

We have compared our results with experimental data : in situ high pressure neutron diffraction measurements. This comparaison has been published in last july (Phys.Rev.B 90 024206 (2014)). Two oher publications are in progress.

Main key facts (for instance publications / pri ces / oral presentations)

I have participated to 4 internation meeting :

- 2013 a poster session at the 12th Non-Crystalline Matériaux conference (Trento)
- 2013 20 minutes oral presentation at the 7th Internation Discussion Meeting on Relaxations in Complex Systems (Barcelone)
- 2014 20 minutes oral presentation at the Glass and Optical Materials Division (Aix-La-Chapelle)
- 2014 20 minutes oral presentation at the Borate and Phosphate Conference Glasses (Prague)