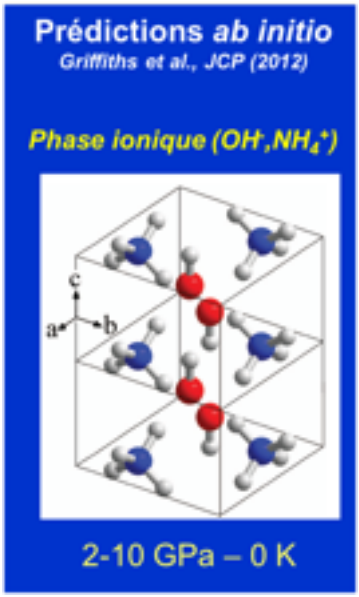
Labex MATISSE

Axe 5

« H_2O/NH superionic compounds at mild conditions? »

Cailong LIU (Post-doctorate)



Hosting laboratories, teams and and thesis supervisors names:

1. IMPMC, équipe Physix, Sandra Ninet
2. INSP, Fabio Finocchi

Research project (10 lines)

This post-doctorate project is focussed on the experimental investigation of the properties of ice mixtures H_2O/NH_3 under high pressure. This project aims at answering fundamental questions regarding the evolution of the hydrogen bonds, self-ionization and onset of superionicity in these simple molecular ices, with relevance to condensed-matter physics and applications in planetary sciences and material sciences. The first objective was to investigate the high-pressure solid phases of the 1:1 NH_3:H_2O compound (ammonia monohydrate, AMH) and determine whether it evolves towards an ionic solid as predicted. The second objective is to couple high temperature with high-pressure studies of NH_3/H_2O mixture to find evidence for the existence of a superionic phase. Superionic states of pure water and pure ammonia have been evidenced around 60 GPa at high temperature (700-1000 K). These phases are excellent proton conductors. The question is now whether this superionic state can also exist in ice mixtures and if it is stable at milder P-T conditions, as suggested by our ab initio MD simulations.

Scientific results & impacts

We have demonstrated that the AMH molecular solid *does* self-ionize at pressures above 7.5 GPa to form an ammonium hydroxide solid (NH_4^+, OH-). We have shown that the structure of this ionic phase differs from the predicted one. Remarkably, the transition pressure is 20 times lower than the ionization pressure observed by our group in pure ammonia (150 GPa) We have also observed that this ionic phase is stable up to 80 GPa, and in a wide temperature range (5K- 300K). In parallel, we have been setting up impedance spectroscopy experiments in the diamond anvil cell to extract a measure of the ionic conductivity under pressure.

Main key facts

These results have been exposed in an oral presentation at the Soleil User's meeting in 2015 and a manuscript is under preparation (Cailong Liu, S. Ninet et al.)

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