

Internship proposal 2011-2012

Laboratory: Institut de Minéralogie et de Physique des Milieux Condensés (IMPMC)

Address: IMPMC Campus Jussieu – 4 Place Jussieu – 75005 Paris, France

Laboratory director: Bernard Capelle



Internship supervisor: A. Marco Saitta (Professeur)

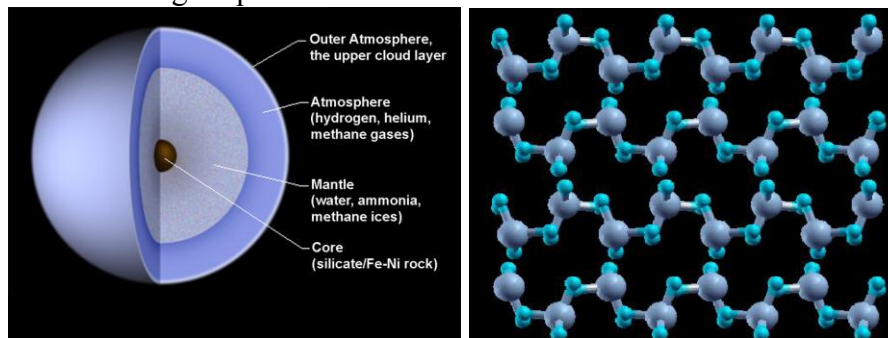
Phone: +33 1 4427 2244

e-mail: marco.saitta@impmc.upmc.fr

Ionic and superionic ammonia ice(s)

Scientific project: Much like water, ammonia is a prototypical molecular H-bond compound whose structure and transport properties at extreme conditions of pressure and temperature are highly relevant in astrophysics and planetary science, as well as in fundamental physics. Superionic phases of ammonia and water were theoretically predicted in a milestone paper, possibly linked to the Jovian planets magnetic fields. Superionicity is a spectacular exotic state of matter where the standard concepts of solid and liquid are baffled, as the system has simultaneously a crystalline (nitrogen) and a liquid (hydrogen) behaviour.

We recently achieved the first combined experimental and theoretical observation of superionic ammonia ice, at much lower temperatures than predicted. This work, currently under publication in a prestigious journal, suggests that yet more exotic forms, such as the recently proposed ionic lamellar phase, could be observed at higher pressure.



We propose to explore the unknown high-pressure/high-temperature regions of the ammonia ice phase diagram, in order to discover new phases having even more interesting properties, and at the same time provide a microscopic interpretation of the upcoming experimental results from our coworkers.

Techniques in use: Ab initio Molecular Dynamics Simulations, Density-Functional Theory

Applicant skills: Basic computer and programming skills, strong motivation, interest in close collaboration with experimentalists.

Granted internship: yes (398.32 €/month)

C'nano IdF laboratory (France only): yes

Possibility for a thesis: yes (type of grant: Ministère, LabEx MATISSE)