


Internship proposal 2010-2011

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Ammonia at high pressure: an ionic compound ?

Scientific project :

Pressure is a useful parameter for material synthesis with growing use in research and industry. One of the most famous and important example is the synthesis of ammonia from its elemental constituents (Haber-Bosch process) whose industrial production has had a major impact on the world food supplies. In this case, modest pressure (100 bar) was used to enhance a chemical reaction according to the Le Châtelier principle. At present, much higher pressures can be routinely obtained in the laboratory (up to several millions of bar), which directly affect the chemical bonds and has allowed the synthesis of new materials with useful properties : ultra-hardness, high Tc superconductivity, energetic compounds...

In condensed phases of water and ammonia, molecular covalent bonds coexist with hydrogen (H) bonds. In water ice, it has been shown that the effect of high pressures is to strengthen the H-bonds at the expense of the covalent ones. When both bonds become comparable in strength, the protons delocalize to the centre of the bond ('symmetrization') and water ice can then be described as two sublattices of oxygen and hydrogen ions. This phenomena was predicted and observed at about 0.6 Mbar. In ammonia, the geometry of H-bonds is more complex and no symmetrization has been observed up to 1.2 Mbar. But a recent theoretical study has predicted that ammonia too will form an ionic solid, composed of alternate layers of NH_4^+ and NH_2^- ions, at pressures around 1 Mbar.

During this internship we propose to realize high pressure experiments to look for evidence of this new phase of ammonia. We will start by studying the phase diagram of binary mixtures of ammonia and helium in a diamond anvil cell, in order to find a good sample topology to perform Infrared (IR) spectroscopy experiments. These IR experiments will be performed on a FTIR instrument, either at IMPMC for initial characterization or at the SOLEIL Synchrotron (SMIS Beamline) for the very-high pressure experiment.

Techniques in use : Diamond anvil (high pressure) cell, Raman and Infrared spectroscopy

Applicant skills : solid background in condensed matter physics, motivation for experimental physics.

Granted internship : yes (_400_€month)
C'nano IdF laboratory (France only) : yes
Possibility for a thesis : yes (type of grant : UPMC)