'Physique et Chimie des Matériaux' – ED 397 – année 2022

PhD project for funding, to send by 28/02/2022 to

nadine.witkowski@sorbonne-universite.fr under PDF form « acronyme labo_nom PI.pdf »

Research unit (full name + acronym) : Institut de Mineralogie, de Physique des Matériaux et de

Team if applicable : PHYSIX

Address : 4, place Jussieu, tour 23, BP 115

Project leader (PI): Sandra NINET HDR? no Position : Lecturer SU

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Nber of phD under supervision 0 Participation to supervisor training? no Year

Co-supervisor : Stefan KLOTZ HDR? yes Position : Researcher CNRS

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Research unit : UMR7590

International co-supervision ? No

Keyword 1 : High pressure Keyword 2 : ices

Keyword 3 : Hydrogen bond Keyword 4 : superionicity

Select co-funding programme if applicable : select

Project title : Ice mixtures (H2O,NH3,CH4) under extreme pressure and temperature conditions

Project Description :

The interior models of the Jovian planets and their satellites rely on a set of observables (radius, mass, gravitational moments, images of the surface, data on magnetic fields, chemical compositions of the atmosphere...) collected during long and costly space missions. For Uranus and Neptune, the relevant systems are mixtures of the so-called "planetary ices", i.e. solid water (H2O), ammonia (NH3) and methane (CH4), as these are the major components of these bodies. Indeed, the most widespread interior models assume a three-layer structure composed of a rocky core, an icy mantle (mainly composed of dense and hot water, ammonia and methane) and an external atmosphere. The properties of the intermediate icy layer is of particular interest as the peculiar magnetic fields measured by the Voyager II spacecraft could be due to the existence, at high P-T conditions, of a protonic conductive states of ice (called superionic ice). Unfortunatly, up to now, the exact composition of the icy layer is poorly constrained and experimental data on the equation of state (EOS), chemical and transport properties of the icy mixtures at the interiors conditions are still lacking. It is therefore crucial to obtain by experiment precise information on these mixtures for various compositions and over a large range of pressure (P) and temperature (T) conditions to constrain the planetary interior structure.

Our group has a large expertise in the study of ices (and more generaly materials) under extreme P-T conditions. For example, we revealed the existence of new phases of pure ammonia [1-5] and water [6] with "exotic" properties, such as superionicicity, ionicity and metallic conduction [1-5]. In the last years, we have extended our investigations to ammonia/water mixtures [7,8] and demonstrated that these exotic phases also exist in the mixed compounds.

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The goal of this PhD project is to study the ternary mixtures H_2O/NH_3/ CH_4 under high (P,T) conditions as these mixtures are those expected in the icy mantle of giant planets and satellites. In particular, we seek to understand the influence of methane CH_4, which does not hydrogen bond to other molecules contrarily to water and ammonia, and determine if its presence stops or not the proton transfer mechanisms which leads to ionic and superionic states.

To cover and explore the whole P-T domain of the planetary conditions, two types of compression techniques will be used: at IMPMC, on one hand, static high pressure experiments (Raman, IR, XRD) will be performed in diamond anvil cells to investigate the phase diagrams in the range [1-100 GPa ; 300 - 4000 K] and highlight the existence of new exotic phases. Neutron diffraction and quasi elastic incoherent neutron scattering experiments in Paris-Edinburgh Press will be performed to determine the positions of hydrogen atoms and their dynamics. Dynamic compression up to 500 GPa-10000 K will be done in collaboration with Alessandra Ravasio (LULI at Polytechnique), expert in laser-generated shock compression, to reach the relevant (P,T) conditions of the inner layers of Jovian planets and access the transport properties and equation of state.

The subject is highly plurisdisciplinary (Physics, planetary sciences, material sciences) combining in lab experiments (optical spectroscopies, x-ray diffractions, transport measurements) with experiments on large-scale facilities (synchrotrons, neutrons, XFEL, laser megajoule).

The interested candidate should have a strong background in materials science and solid state physics and a strong motivation for experiments.

Rerences :

[1] S. Ninet et al., PRL. 108, 165702 (2012)
[2] S. Ninet et al. PRB 89, 174103 (2014)
[3] J.-A. Queyroux et al., PRB 99, 134107 (2019)
[4] J.-A. Queyroux et al.. PRB, 100, 224104 (2019)
[5] A. Ravasio et al, PRL, 126, 025003 (2021)
[6] J.-A. Queyroux et al, PRL 125, 195501 (2020)
[7] C. Liu, A, et al. Nature Comm., 8, 1065 (2017)
[8] H. Zhang et al. J. Chem Phys. 153, 154503 (2020)