PhD position opening (October 2023)

Title: Theoretical modelling of solid-state batteries

Keywords: Batteries, solid electrolyte, electrode, *ab initio* molecular dynamics, Solid-state quantum calculations

Scientific Context

Nowadays, electricity storage is of paramount importance, notably in the context of Greenhouse effect and carbon footprint reduction. From this point of view, the increase of battery efficiency and power has attracted a great deal of attention. The challenges to be met are numerous and require a better understanding of the materials involved (electrodes and electrolytes) as well as the device interfaces.

The main objective of this thesis is to theoretically investigate all-solid-state batteries based on Lithium or Sodium. This technology has become reality since the discovery of electrolytes exhibiting high ionic conductivities that were comparable to liquid ones. Such approach offers various advantages due to their better electrochemical stability and energy density (exceeding Li-Ion batteries by more than 50%). However, instabilities at the interfaces or dendrites formation at the anode lead to degradation of the performance and/or lifetime of this type of all-solid-state batteries.

The main stages of the thesis will consist in quantum modelling based on density functional theory (DFT). More precisely, the positive electrode will be investigated by means of periodic codes such as VASP, CASTEP and WIEN2k. The atomic scale structure of glassy electrolytes will be characterized using ab initio molecular dynamics within the Car-Parrinello formalism. Fig 1. contains the glassy structure of a typical LIPON-type electrolyte at room temperature and exhibits the PO_xN_y (x+y=4) interconnected tetrahedras. The understanding of the interfaces evolutions processes will be also considered in a second step. All the theoretical results willl be confronted to experimental data (NMR and vibrational spectra specifically) acquired during experimental investigations performed by the Glass & Ceramics team of the Rennes Institute of Chemical Sciences (ISCR).

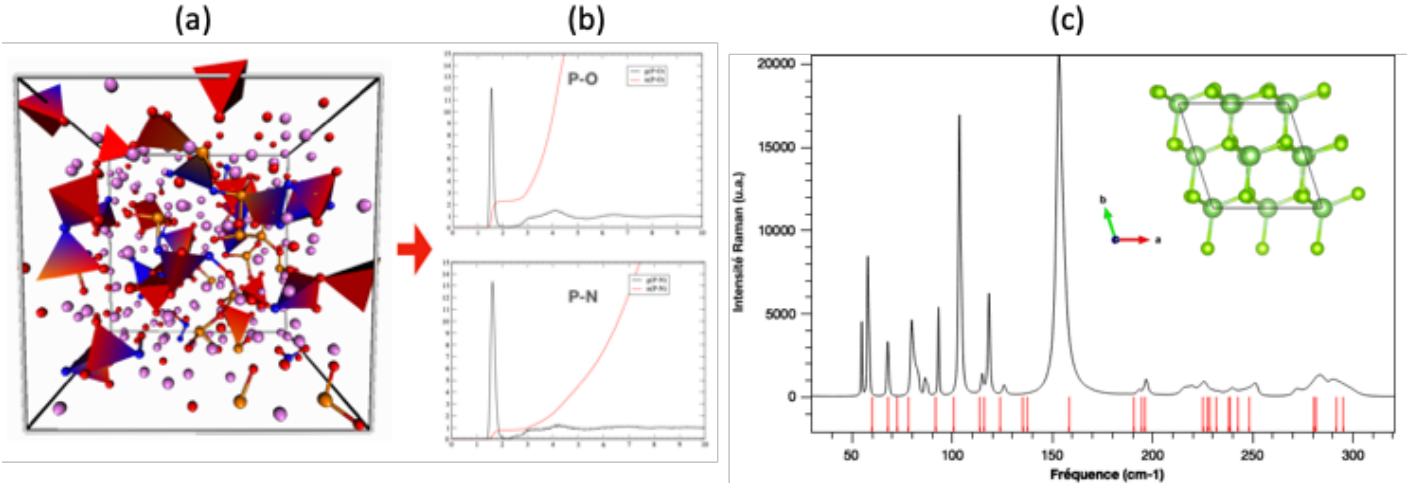

Fig. 1: (a) Structure of a 333 atoms LiPON cell@1300K; Li (pink); P (orange); O(red), N(blue) and (b) selected radial distribution functions (black line) together with their respective integration (red line). (c) Comparison of an experimental Raman spectrum (black curve) of Ga_2Se_3 with the DFT frequencies (red lines) calculated using GGA functional.

Laboratory - Inorganic Theoretical Chemistry Team (CTI)

The PhD student will work in the *Inorganic Theoretical Chemistry* team of the *Rennes Institute of Chemical Sciences*. The CTI team gathers several theoreticians (14-5 permanent staff members, 15 students) with complementary skills in theoretical chemistry but also physics, working with a broad set of quantum chemical tools, ranging from high precision *ab initio* wavefunction-based calculations to fast semi-empirical methods. The studied systems in CTI are diverse, including isolated species, bulk materials and surfaces, mainly of high experimental and societal interest. This has led to fruitful joint collaborations with experimentalists from ISCR as well as major national and international groups. The team is also strongly involved in the collective effort made by the French community of theoretical chemists at the national level, in the quest of bridging the gap between state-of the art quantum tools and real-life applications. The CTI team thus provides a stimulating scientific environment, also offering regular team meetings, invited seminars as well as visitors internationally recognized. Local and national computing means are available for the purposes of the scientific projects.

Candidate Profile

The PhD Student will be in charge of the DFT calculations in order to obtain in silico samples of electrolytes and electrodes (in crystalline and glassy state). He will compute elastic and vibrational (phonons) properties, as well solid-state NMR spectra. ***The selected student will have a solid experience in solid state science and DFT calculations.*** *During the thesis, he will be involved in regular meetings (discussions and seminars) with experimentalists. Therefore, good communication skills in English and French would be a plus. From a general point of view, good chemical physics knowledge and scientific curiosity are mandatory.*

Application

The PhD project will start in October 2023. Applications are already open and candidates shall contact both supervisors by e-mail, with a CV and a motivation letter, including clear description of previous Master internship(s).

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