ECOLE DOCTORALE DES SCIENCES CHIMIQUES - ED 040

Proposition de sujets de thèse pour la rentrée 2024 / 2025

Titre de la thèse	Characterization and modelling of ionic diffusion in Halides as solid electrolytes for Li-ion batteries
Descriptif du sujet (10 lignes maximum)	For energy storage, nowadays, Li-ion battery is the major technology for mobility applications, but suffers from safety issues with standard liquid electrolytes. The development of all solid-state batteries has become a major challenge in the field. Among several solid electrolyte candidates, halides appeared recently really promising candidates, as they exhibit good ionic conductivities (~10^{-3} S/cm-1) and wide electrochemical stability window. In this project, using ab initio calculations, we aim to focus on the understanding of the ionic diffusion mechanisms in the lattice depending on the composition and atomic local arrangement. Several Li_3YX_6 materials will be studied depending on the nature of X- (F-, Cl-, Br- or a combination of those ions). Y^{3+} partial substitution by metal ions with higher oxidation state will also be considered as a way to increase ionic conductivity by introducing metal vacancies ($Li_3M_{1-x}\square_xX_6$). Due to the expected disorder in the structures, large cells will have to be considered for the simulations. The use of the large scale DFT code CONQUEST will therefore be preferred. The theoretical results will be discussed together with the experimental local structure of the materials investigated by NMR spectroscopy and the experimental ionic diffusion measurements obtained by NMR and impedance spectroscopy.
Compétences souhaitées (nom du DEA, ou MASTER, etc…)	Material Sciences, Solid State Physics, Physical Chemistry, Computational Sciences, Quantum Physics and Chemistry, Density Functional Theory
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