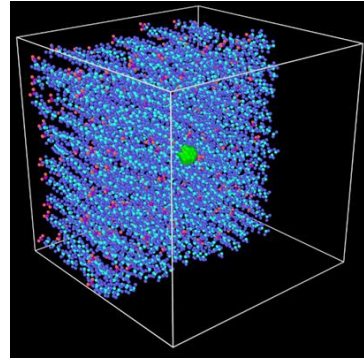


PhD studentship: **Multiscale modeling of lithium transport in solid and hybrid Li-ion electrolytes and their interfaces**

A 3-year studentship is available at **CEA-Grenoble**, from **October 2020**, for the theoretical and computational design of new-generation electrolytes for Li-ion batteries, towards obtaining a PhD degree.

Description of the thesis project:

The energy density limitations of current Li-ion batteries constitute an obstacle for the widespread replacement of fossil-fuel vehicles by electric ones. In coming years current generation-3 batteries will give place to new, all-solid-state batteries, with a much higher energy density. Theoretical and computer-based modeling of new materials for this generation-4 is an essential part of these upcoming developments, in order to understand the physics, and optimize the battery performance and safety from an atomic-level knowledge of the electrode and electrolyte materials. Novel approaches in machine-learning-augmented *ab initio* techniques to be used in this thesis can provide essential insights into the possibilities and limitations of the new material concepts currently being explored.



We will carry out multiscale simulations of the ion-conduction properties of hybrid polymer electrolytes with embedded ceramic nanoparticles. The addition of nanoparticles in electrolyte polymers has been shown to significantly enhance their Li-mobility. However, the microscopic physical reasons for this enhancement are not yet understood, and no atomic level or multiscale *ab initio* modeling has yet been undertaken on these systems. This thesis aims to *theoretically elucidate* the currently unknown transport mechanisms of Li in hybrid polymer/ceramic electrolytes, and to *quantitatively predict* performance and aging properties related to these mechanisms.

This research will be carried out at the Computational Materials Physics group of CEA-Grenoble, <https://sites.google.com/view/natalio-mingo/home>, under the supervision of A. van Roekeghem, S. Mossa, and N. Mingo.

To apply:

Candidates should have a master degree in condensed matter physics or related field, and be proficient in computer programming. Please send **CV and motivation letter** as soon as possible to natalio.mingo@cea.fr