PHD Proposal at University of Montpellier - Institut Charles Gerhardt

Theoretical Design of High-Energy-Density Materials for Batteries

In the field of electrochemical energy storage, Li-Ion batteries have conquered the market of portable electronics as the leading technology to store high density of energy in a small volume. However, to meet the ever-increasing energy demand of our planet and make it possible large-scale applications such as electric vehicles, the performance of the batteries still needs to be improved. Over the past 20 years, intensive researches have focused on increasing the energy density of Li-Ion batteries, which is mainly limited by the positive electrode in today's batteries. This research has led to the emergence of a new class of transition metal oxides with improved energy density thanks to a cumulative cationic and anionic redox activity. Unfortunately, these materials suffer from poor cycling performance as well as potential hysteresis between charge and discharge cycles, which hinder their commercialization. Understanding the microscopic phenomena at the origin of these thermodynamic instabilities is essential to envision these materials for industrial large-scale applications. In this context, theoretical chemistry is the tool of choice to rationalize the structural and electronic mechanisms underlying the Li-driven electrochemical reactions taking place in charge and discharge and to propose alternatives to current materials. [1] To this aim, electronic structure calculations based on the formalism of the density functional theory will be implemented to establish direct links between the material chemistry and its electrochemical response. Once established, not only this link will allow to target the best possible candidates among those already reported in the crystallographic databases, but will also provide our experimental collaborators with rational recipes for the design of new materials with improved performance.

[1] Mouna Ben Yahia, Jean Vergnet, Matthieu Saubanère and Marie-Liesse Doublet « Unified picture of anionic redox in Li/Na-ion batteries" Nat. Mater. 2019, 18, 496-502

We are looking for a motivated candidate with solid training in materials chemistry and / or physics and / or in general chemistry-physics and willing to get involved into high-impact research topic in strong collaborations with solid state chemists. Skills in programming and in quantum-based methods will be an added-value, although it does not constitute an absolute requisite.

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Keywords: Energy storage, Chemical bond analysis, periodic and molecular DFT calculations, Electronic structure, Li-Ion Batteries, Anionic redox