CYCLE DE CONFÉRENCES DE CHIMIE

Avec le concours de : Université Clermont Auvergne
INP Clermont Auvergne

Lundi 13 novembre à 14 h (hors cycle)

Bibliothèque UFR de Chimie (Chimie 7, RDC, site des Cézeaux)

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Links between synthesis, composition, and performance in battery materials from magnetic resonance spectroscopy

Batteries have transformed our daily lives and hold the key to a low carbon future. Yet, current Li-ion chemistries are approaching their theoretical performance limit. Remarkably, we continue to rely on a limited subset of Li-ion battery materials — most commercial cathodes derive from $LiCoO_2$ developed in 1980 — that cannot meet our ever-growing need for energy storage. The development of more sustainable, energy dense, and safer batteries hinges on designing new cathode chemistries and crystal structures that depart from the traditional layered lithium transition metal oxides, as well as non flammable solid electrolytes.

In this talk, I will present our work combining solid-state NMR, first principles simulations, and other advanced tools to relate synthesis, structure, and properties in various classes of battery materials. For example, our work on Li-ion rocksalt oxyfluoride cathodes emphasizes the importance of $^{7}Li/^{19}F$ solid-state NMR to determine the true composition of such systems and establish robust materials design rules, and introduces a new, rapid and energy-efficient synthesis procedure to obtain those materials. I will also present our work on weberite-type Na-ion cathodes, which offer an attractive alternative to the lithium technology, particularly when combined with Earth-abundant redox-active species such as iron. Finally, I will discuss our work on Li- and Na-ion conducting rocksalt halide solid electrolytes, highlighting their high propensity for polymorphism and for the formation of planar defects, with resulting structural and ion conduction properties that can be modulated by changing the synthesis conditions.

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