UNIVERSITY OF CALIFORNIA, IRVINE

Department of Materials Science and Engineering

From Order to Disorder: NMR Insights Into Ionic Conduction in Battery Materials

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Abstract: Nuclear magnetic resonance (NMR) spectroscopy provides detailed insights into the working principles of ionic and mixed conductors used in rechargeable battery applications. Notably, NMR is sensitive to crystalline, disordered or even amorphous phases that arise during electrochemical cycling, and can provide atomic-level structural information, as well as insights into the dynamics of ion motion. In this talk, I will present our recent work on Li- and Na-ion conducting rocksalt halides and Li-conducting polymeric ionic liquids. Using a combination of electrochemical impedance spectroscopy (EIS), solid-state NMR, pulsed field gradient NMR (PFG-NMR), NMR relaxometry, and first principles calculations, we provide a multiscale understanding of ion diffusion processes and link these findings to local structure features, crystallinity, and materials synthesis/processing conditions.

Bio: Raphaële Clément is an Assistant Professor in the Materials Department at the University of California Santa Barbara (UCSB). She received her Ph.D. in Chemistry in 2016 from the University of Cambridge, working under the supervision of Prof. Clare Grey. Her doctoral work focused on the study of layered sodium transition metal oxide cathodes for Na-ion secondary batteries. She then joined the group of Prof. Gerbrand Ceder at the University of California Berkeley (UC Berkeley), focusing on cation-disordered rocksalt oxyfluorides for Li-ion battery applications. She joined the Faculty at UCSB in 2018. Her primary research focus is the development and implementation of magnetic resonance techniques (experimental and computational) for the study of battery materials and beyond, with a strong emphasis on *operando* tools. She recently received the NSF CAREER award and is an Associate Editor for *Battery Energy*, a new open access journal by Wiley.