Data driven exploration of electrochemical reaction networks: application to electrolytes degradation path-ways.

Scientific context: A fully funded PhD position is available for candidates with a strong background in chemistry, physics, or materials science. The successful candidate will join the IPREM institute (https://iprem.univ-pau.fr/) at the University of Pau and Pays de l'Adour (UPPA). The current offer lies in the context of the REACTIF joint research program between IPREM, the iC2MC joint laboratory, and Saft (https://saft.com/), a pioneering company specializing in innovative electrochemical storage devices.
The REACTIF project, Deciphering REACtion Mechanisms at Electrode/Electrolyte Interfaces: a Key Step toward High-PerFormance Lithium-Ion Batteries, focuses on developing advanced and transdisciplinary methods integrating analytical chemistry, computer simulations, and chemical-physics surface characterizations to investigate and improve the performance and durability of lithium-ion batteries (LIBs). A key challenge in LIB technology is the formation and evolution of interfacial layers along battery charge and discharge operations. More precisely, the Solid Electrolyte Interphase (SEI) at the anode and the Cathode Electrolyte Interphase (CEI) at the cathode. These nanometric layers, formed during electrochemical cycling, play a crucial role in battery stability but are also central to aging phenomena and performance loss. Within the REACTIF project, this PhD work will focus on deciphering at the molecular level the chemical processes that govern the formation and composition of SEI and CEI.

Description of the research project: This PhD offer aims at developing innovative computational methods for exploring Chemical Reaction Networks (CRNs). These networks provide a holistic view of complex chemical processes, bridging the results obtained from experimental and theoretical data. The focus will be on building and analyzing CRNs that describe the (SEI) formation and electrolyte degradation. These processes are difficult to characterize due to the high density and diversity of chemical species and reaction pathways involved under electrochemical conditions. New algorithmic tools will be used to identify key species and critical reaction mechanisms. This part will be achieved by leveraging an existing collaboration with the University of California, Berkeley, and the iC2MC joint research lab. A major challenge will be to incorporate accurate thermodynamic and kinetic data into the CRNs including chemical elements or new molecular species that are part of the electrolyte composition. Complementary quantum chemistry calculations (molecular and solid-state) will be used to evaluate activation barriers, and transition states for key reactions.
This work will be tightly coupled with the results obtained from high-resolution mass spectrometry (HRMS) data from other parts of the REACTIF project. Molecular identifications provided by HRMS will serve as key constraints to refine and validate the CRNs iteratively. Conversely, simulations results will help in the assignment of the experimental signals the whole contributing the enhance the understanding of the SEI compositions.

Candidate profile: The successful candidate should old a Master degree (Maste 2 in France) or equivalent in Chemistry, material sciences or Chemical-Physics with a strong background in computational chemistry. S/he should be particularly motivated to work in an environment with national and international collaborations, in contact with industrial partners and at the interface of several disciplines. English speaking and computer sciences skills are required (Python, HPC calculations). A previous experience in quantum chemistry, molecular simulations, code development would be appreciated.

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