Séminaire

Mardi 25 mars 2025 à 10h30

Amphithéâtre Henri Benoît

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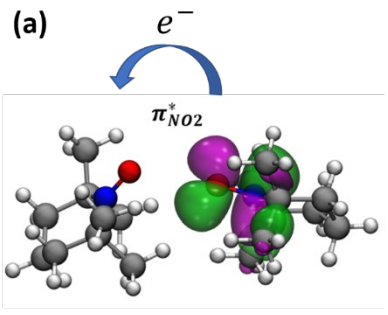
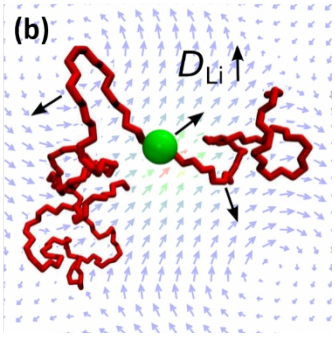
Molecular Modeling of Battery Materials – From Electrons to Polymers

Driven by the demand for batteries as mobile and stationary energy storages, current research focuses on identification and characterization of both electrolytes and active materials. This talk will focus on how molecular modeling techniques can support or even guide experimental investigations. In the first part, I will show how first-principles methods can be utilized to study the thermodynamic and kinetic properties of electron transfer processes in organic redox-active materials employed in redox flow batteries or polymer-based batteries. Here, the mutual inter- and intramolecular interactions between monomers give rise to highly diverse electron transfer rates due to subtle differences in orbital overlap. In the second part, I will present a hydrodynamic theory describing dynamical ion correlations in electrolytes [1], which are relevant to compute ionic conductivities from Molecular Dynamics simulations, and can thus be utilized to rationalize the performance of electrolytes. Remarkably, although this framework has originally been derived for liquids, it turns out that it holds for polymers too, and can hence be leveraged to design strategies to overcome current limitations [2].





Schematic illustrating (a) the electron transfer between two redox-active monomers and (b) the hydrodynamic flow field in a polymer electrolyte.

[1] Diddens *et al.*, *J. Chem. Phys.* **2023**, 158, 154112

[2] Atik *et al.*, *Angew. Chem. Int. Ed.* **2021**, 60, 11919

Les personnes souhaitant rencontrer D. Diddens sont priées de prendre contact avec Albert Johner.