Understanding the electric double-layer from molecular dynamics

Mathieu Salanne*

[a]*Sorbonne Université, CNRS, Laboratoire PHENIX, Paris, France*
[b]*Institut Universitaire de France, 75231 Paris, France*

**mathieu.salanne@sorbonne-universite.fr*

Applied electrochemistry plays a key role in many technologies, such as batteries, fuel cells, supercapacitors or solar cells. It is therefore at the core of many research programs all over the world. Yet, fundamental electrochemical investigations remain scarce. In particular, electrochemistry is among the fields for which the gap between theory and experiment is the largest. From the computational point of view, this is due to the difficulty of combining a realistic representation of the electrode electronic structure and of the electrolyte structure and dynamics. Over the past decade we have developed a classical molecular dynamics code that allows to simulate electrochemical cells [1]. The method, which was first applied to the study of supercapacitors [2], provides a microscopic insight on the structure of the electrolyte in the electric double-layer, even for concentrated electrolytes which cannot be treated using classical theories. It also allows to study the adsorption of the ions inside electrified nanomaterials such as MoS_2 [3] or nanoporous carbons [4]. More recently, we have extended the scope of these studies to the case of electrocatalysis [5].

References:
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