Adsorption and structuring processes at single-crystal electrode | ionic liquid interface – insights from simulations and *in situ* studies

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Ionic liquids (ILs) have established their significance due to their numerous applications in novel energy storage and conversion devices [1]. Currently, the focus has been mainly on the characterization of pure ILs interfacial behaviour, while the adsorption of organic molecules from IL electrolytes has attracted significantly less attention. The self-assembly of organic molecules into ordered rows and wires on the electrode's surface offers various options for surface functionalisation. The formation of nanostructures also provides insights into the subtle interplay of various interactions between the electrode, organic adsorbate, and the electrolyte[2].

The given presentation focuses on the studies of the properties and structure of electrode | IL electrolyte in the case of C[3], Au(100)[4], Sb(111)[5], and Bi(111)[6] model electrodes. The combination of both experimental and computational techniques has allowed us to: study the capacitance-structure relationship by relating the characteristic peaks to the reorganization of the IL layers, provide a multifaceted description of the 4,4'-bipyridine adsorption, obtain insight into the interplay between different interactions in IL, and highlight the differences in aqueous and IL electrolyte interfacial behaviour.

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