INVESTIGATING THE HYSTERESIS OF DIFFERENTIAL CAPACITANCE AT THE IONIC LIQUID–GOLD INTERFACE USING MD SIMULATIONS

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Understanding the properties of the electrode-electrolyte interface and its response to the applied electric field is important in designing more efficient capacitors and actuators. In these devices, the electrical double layer (EDL), formed at the interface, has a key role. Ionic liquids (ILs) have been studied as possible electrolytes for supercapacitors due to their unique properties, such as large electrochemical stability [1]. Modelling the interfaces between electrode and IL using molecular dynamics (MD) gives fundamental atomic-level insight into the IL's complex EDL structure [2].

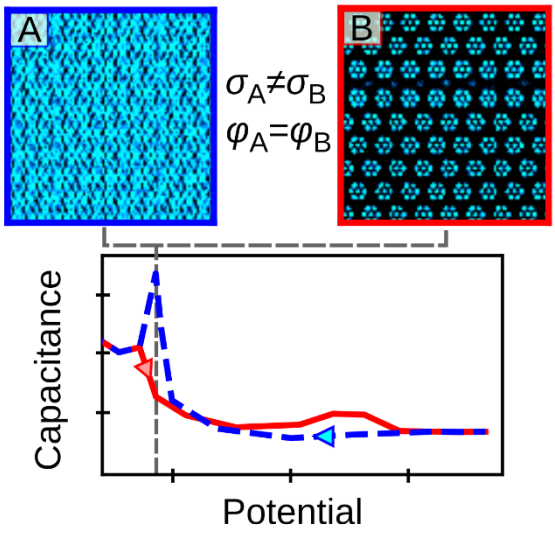

Figure 1. The dependence of IL's interfacial structure on the potential scan direction.

In this study [3], we investigated the interface between 1-butyl-3-methylimidazolium hexafluorophosphate IL and Au(111) electrode using the MD to study the hysteresis of differential capacitance due to the scan direction of applied potential. The results of the simulations show the formation of two different ionic liquid interfacial structures, which screen the electrode's charge differently as the cause of the hysteresis.

Acknowledgments:

This work was supported by project UID/QUI/50006/2020 (LAQV@REQUIMTE) with funding from FCT/MCTES through Portuguese national funds, by the Estonian Research Council grant PSG249, and by the E.U. through the European Regional Development Fund under project TK141 (2014- 2020.4.01.15-0011).

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