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Theoretical DFT study of the electrified Au(111) | EMIMBF₄ ionic liquid interface using cloud computing

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Growing interest to the chemistry and physics of room temperature ionic liquids (RTIL) has recently reached electrochemistry, for which RTILs appeared to be very promising electrolytes: nonvolatile and non-destructive under high voltages [1]. Attempts to find the ways to apply RTILs as solvent-free electrolytes in supercapacitors and batteries has triggered a number of new theoretical, experimental and simulation studies of the capacitance at the electrified metal | RTIL interface (see Refs. in [2]). In the presented work the adsorption of EMIm⁺ and BF₄⁻ ions was studied by means of periodic density-functional theory calculations. The first aim of the study was to investigate the charged Au(111) | 1-ethyl-3-methylimidazolium tetrafluoroborate (EMImBF₄) interface. We focused on local ion–surface interactions, which are ignored in most molecular dynamics simulations and are poorly studied. To elucidate the importance of van der Waals interactions in case of EMIM⁺ adsorption at Au(111) we applied vdW-DF functional [3]. A model developed in Ref. 4 was applied in order to estimate the interfacial capacitance of the BF₄⁻ adlayer at Au(111) [5]. Most recent calculations mimic EMImBF₄ crystalline layer at uncharged Au(111) surface and represent the second aim of the work, which is to test cloud computing applicability for quantum chemical computations. We demonstrate the results of calculations held on SciCloud using Desktop to Cloud software developed in the University of Tartu (Estonia) [6]. Prospects for cloud computing are discussed in relation to computational electrochemistry.

References

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