Quantitative modeling of hybrid interfaces for future electronics and energy storage applications

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The main objective of this PhD project is a detailed study via advanced simulation techniques, of the integration of ionic gels in next-generation electronic devices in large-area 2D Quantum Materials (la-2DQM). To date, ionic liquids (ILs) are routinely used as a gate for three-terminal devices and have led to major experimental findings such as the superconductivity induced by an electric field. Yet, integrating these composed materials into real devices is challenging because ILs are in a liquid state at the typical operating temperatures. This implies stability problems typical of any fluid phase. To circumvent this difficulty, ionic gels can be conceived on the basis of a targeted IL upon addition of a polymer able to induce a gelification. In this context, we propose to focus on the integration of these ionic gels into la-2DQM device via molecular modeling, backed and supported by experiments. The scope of the PhD thesis project will be a precise understanding of the fundamental interactions occurring at the interface between the ionic gels and the 2DQM materials. This crucial information will provide the still lacking insight into this type of interfaces and will pave the route for experiments at a quantitative level not accessible to the qualitative approaches still used nowadays, neglecting the subtle effects of the electronic structure and its modification upon formation of interfaces. The expected results will allow to: (i) establish the relation among the atomic structure, the ionic mobility and the charge redistribution at the 2D surface in the presence and absence of a coadiutaving polymer; (iii) give a roadmap for a computer-aided design of innovative hybrid materials with possibility of covalent-bond driven doping at the interface bewteen ions and semi-conducting materials. For the tasks proposed, dynamical simulations involving molecular motion and chemical reactions will be performed within the density functional theory (DFT) framework [1-6]. These approaches are available in the computer codes CPMD [7] and CP2k [8], for which the supervisor of this thesis is co-developer. The PhD candidate will be formed and trained to the use of these codes, an aspect that will contribute to enrich the knowledge of the student in computer simulations, exploitable also in the rest of his/her professional career either in academy or in industry.

This PhD thesis project will be exploit computational resources available at the HPC facility of the University of Strasbourg and national centers (IDRIS, CINES, TGCC). Moreover, the experience of our team in the development and use of the most advanced techniques and codes will provide a solid background for the formation of the candidate.

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