

Nanoscale analysis of the electrode/electrolyte interface in protic ionic liquids

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In order to limit the emission of greenhouse gases, fossil fuels have to be replaced by renewable resources such as wind and solar energy. Until now, their intermittency is one of the biggest challenges for a complete transition of the energy system. Therefore, a storage system, which relies on electrochemical energy converters and employs the chemical reaction between hydrogen, oxygen and water, could serve as an efficient solution for this problem. In particular for automotive application, the use of polymer membrane electrolyte fuel cells (PEMFCs) is thought as an efficient alternative to combustion engines. However, the overall efficiency of fuel cell cars is still lower in comparison to battery cars, which demands for an improvement of the employed technology.

Today's fuel cell cars operate at temperatures of about 80 °C, which requires a complicated heat and water management system. Hence, it is expected that a significant efficiency improvement can be achieved by increasing the operation temperature above 100 °C. In order to reach this goal, novel electrolytes, which are stable in this temperature range and still allow an efficient proton transport, have to be developed. Hence, we evaluate the usability of protic ionic liquids (PILs) as fuel cell electrolytes. As ionic liquids are matter composed entirely of ions, their electrochemical behavior is fundamentally different from that of aqueous solutions. In particular, the formation of the electrical double layer at the interface between electrode and electrolyte cannot be explained by the classical theories of Helmholtz, Guy, Chapman, and Stern. Instead, one has to take into account that alternating anion and cation layers will form at a charged interface, which will also influence the reactions taking place at the electrode surface and the proton transport in the membrane.

In order to investigate the nature of the double layer experimentally, we employ infrared spectroscopy and atomic force spectroscopy. These experiments confirm that a dense layered structure at the interface is present that not only depends on the electrode potential, but is furthermore influenced by the presence of water in the ionic liquid, which is unavoidable during fuel cell operation. Based on these experimental results, we aim on developing a model for the interface formation by means of density functional theory (DFT) in combination with molecular dynamics simulations, which will be used to select and develop promising material combinations of electrode, ionic liquid and membrane.