Organization and Wetting of $[C_4Mim][Ntf_2]$ Ionic Liquid at the Neutral Sapphire Interface

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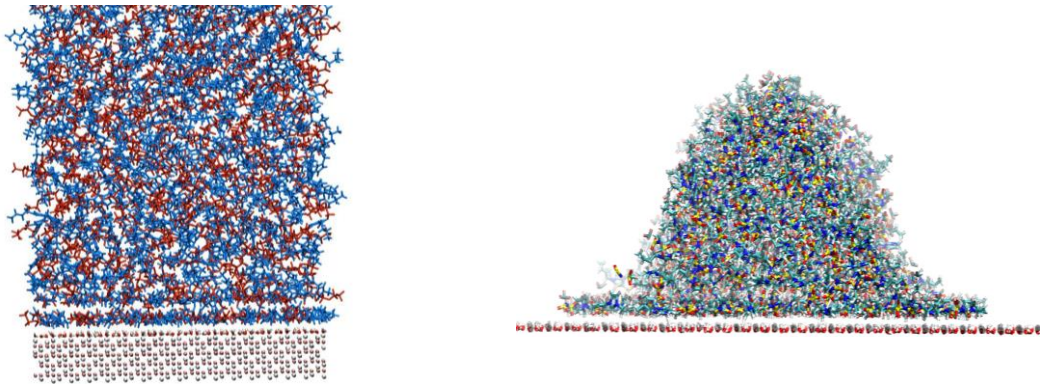

Understanding the molecular-level behavior of ionic liquids (ILs) at IL−solid interfaces is of fundamental importance with respect to their application in, for example, electrochemical systems and electronic devices. [1] In this respect, we employed atomistic molecular dynamics (MD) simulations to investigate the behavior of an archetypical imidazolium-based IL, namely $[C_4Mim][NTf_2]$, at the neutral sapphire interface. [2] This enabled us to describe the nature of the model IL−solid interface in appreciable detail. More precisely, we observed pronounced structural ordering of the IL constituents in the vicinity of the sapphire surface, which, in turn, induces the multidimensional layering of cations and anions. Moreover, we investigated the surface-wetting capabilities of $[C_4Mim][NTf_2]$ by employing cylindrically shaped nanodroplets [3] with three different radii, thereby measuring the contact angle between the IL and the sapphire surface.

[1] T. Welton, *Chem. Rev.* **1999**, *99*, 2071-2084.
[2] Z. Brkljača, M. Klimczak, Z. Miličević, M. Weisser, N. Taccardi, P. Wasserscheid, D. M. Smith, A. Magerl, A.-S. Smith, *J. Phys. Chem. Lett.* **2015**, *6*, 549-555.
[3] J. Driskill, D. Vanzo, D. Bratko, A. Luzar, *J. Chem. Phys.* **2014**, *141*, 18C517.