Imidazolium-based Ionic Liquids under the Magnifier of Molecular Simulations

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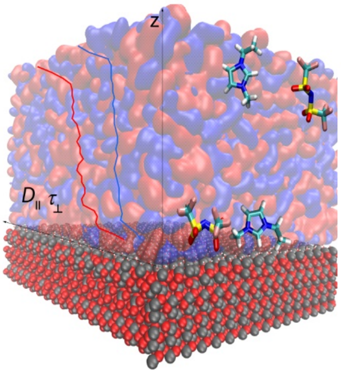

With the aim of understanding the structural organization and dynamic properties related to Supported Ionic Liquid Phase (SILP) catalysts, we present an in-depth study of the [C_2Mim] [NTf_2] ionic liquid (IL). Using classical molecular dynamics (MD) simulations, the IL is considered in three configurations, corresponding to the pure liquid (L), vacuum-liquid-vacuum (V-L-V) and solid-liquid-vacuum (S-L-V) arrangements. In the first part of the study, by combining charges derived from CHelpG, RESP-hf and RESP-b3lyp with charge scaling factors of 1.0, 0.9 and 0.8, we search for an optimum force field (ff) parameterization. This is achieved by benchmarking the static and dynamic responses of the three model systems against experimental data such as self-diffusion coefficients (L), surface tension (V-L-V) and X-ray reflectivity (S-L-V). [1] Consequently, we provide detailed atomic descriptions of the IL at the solid and vacuum interfaces, which are in very good agreement with experimental data such as low-energy ion scattering experiments. [2] We further leverage the extensive data generated to provide evaluation of lateral diffusion coefficients, in the xy plane, and residence times along the z-direction.

[1] N. Vučemilović-Alagić, R. D. Banhatti, R. Stepić, C. R. Wick, D. Berger, M. U. Gaimann, J. Harting, D. M. Smith, A. S. Smith, *J. Colloid Interface Sci.*, **2019**, *553*, 350-363.
[2] N. Vučemilović-Alagić, R. D. Banhatti, R. Stepić, C. R. Wick, D. Berger, M. U. Gaimann, J. Harting, D. M. Smith, A. S. Smith *Data in brief*, **2020**, *28*, 104794.