Investigation of the impact of dissolved H_2 on the surface properties of ionic liquids

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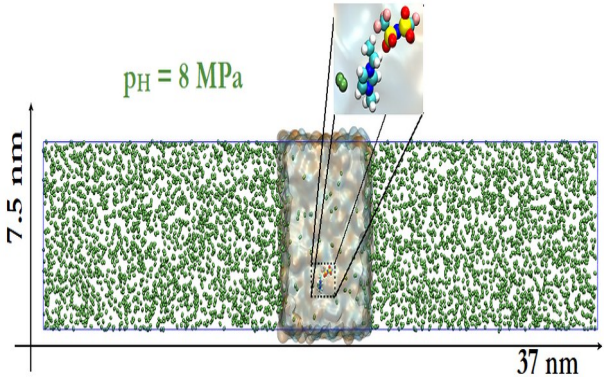
SILP (Supported Ionic Liquid Phase) catalysis technology focuses on obtaining a heterogenised type of homogeneous catalytic systems where a thin film of ionic liquid (IL) containing a homogeneous catalyst is immobilised on the surface of a porous support material, which is commonly employed in hydrogen-involved catalysis systems. The dissolution of small, non-polar molecules of hydrogen in the ionic liquid film resulting in highly asymmetrical system in terms of molecular structures, is expected to have an influence in the thermophysical properties of IL which can subsequently affect the reaction kinetics and ultimately impact the overall reaction rate. In order to understand this influence of dissolved hydrogen on the surface properties of ILs, molecular dynamics (MD) simulations were conducted using GROMACS software in binary mixtures consisting of an ionic liquid (IL) with pressurized molecular hydrogen (H_2),between 298 and 393K over a broad pressure ranging from 1 to 30 MPa. We find that the addition of H_2 results in a decrease in the surface tension of both binary mixtures up to about 6 percent at higher pressures, which is more pronounced at lower temperatures. Furthermore, an enrichment of hydrogen is observed at the liquid-gas interface of these binary mixtures.



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