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Why does the tail matter? Cation alkyl group modulates the interaction of ionic liquids with nano and biomaterials

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Highlights

Molecular dynamics simulations of ionic liquids with 1 and with 2 alkyl groups in the cation show distinct organization and capacity to stabilize nanoparticles and different effects over lipid bilayer

Abstract

Ionic liquids (ILs) have attracted great attention in the last years in applications such as synthesis and stabilization of nanomaterials and as solvents and nanocarriers for drugs. Those applications take advantage of the amphiphilic character presented by several ILs, which is usually due to a cation with one or more alkyl groups. If those groups are long enough, the IL displays nanoscale domain segregation and, for even long tails, mesophases of anisotropic nature. Despite the existence and the effects of those domains being well-known in the pure ILs, their effects over complex bio and nanostructures have been less explored so far. In our group, we were conducting systematic studies of the effect of domain segregation over nanoparticles aggregation and adsorption as well as over the interaction with lipid bilayers by changing the alkyl groups length of CnCm imidazolium-based ILs, where n and m are the length of alkyl groups. In recent work, we showed that the domain segregation in C8C1 provides kinetic stability to nanoparticles (NPs) and also results in a long-order arrangement while C4C1, which doesn't display significant domain segregation, cannot stabilize the dispersion (https://doi.org/10.1021/acsnano.4c04581). The same effect controls the adsorption of NPs over solid substrate: C4C1 results in no long-range force, C8C1 in multiple barriers for the adsorption, and C12C1 in a strong repulsion between the surface and the NP since the later disturbs the long range order of the schematic phase (Figure 1 a-b). The alkyl groups also modulate the interaction with lipid bilayers, which are crucial for the use of ILs for drug delivery or as antibiotics. While C4C1 is soluble in water and the cations display a small tendency to penetrate the bilayer, both C16C1 and C16C16 are insoluble in water. However, C16C16 forms spherical droplets that migrate to the center of the bilayer while C16C1 stays at the surface of the bilayer and removes some lipids (Figure 1 c). Those effects are related to the nature of the portions of the liquids exposed to water.

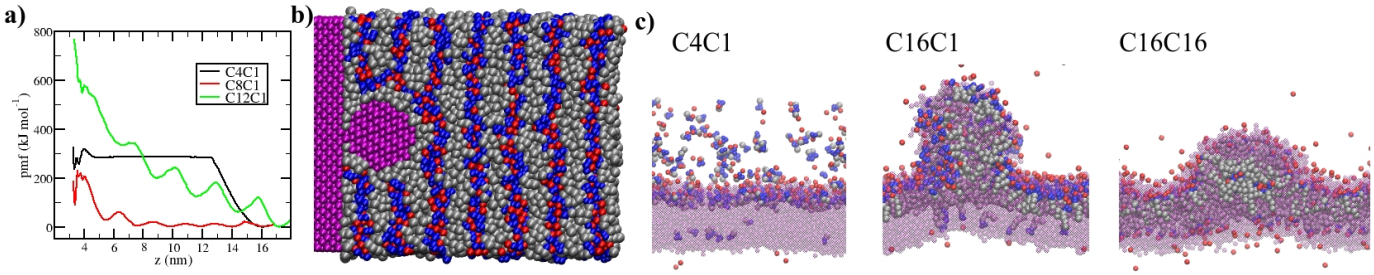

Figure 1 – a) Potential of mean force (pmf) for the adsorption of a hydrophobic NP over solid substrate though thin films of different imidazolium-based ILs. b) Graphical representation of the surface with the adsorbed NP in the presence of C12C1 film. c) Interaction of C4C1, C16C1 and C16C16 with a DPPC bilayer. Colors in b-c: Purple: NP, solid substrate and lipid, Blue: Cation polar head, Gray: Cation apolar tail, Red: Anion.

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