ChemSusChem

Supporting Information

Ionic Liquids as Extractants for Nanoplastics

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Supporting Information

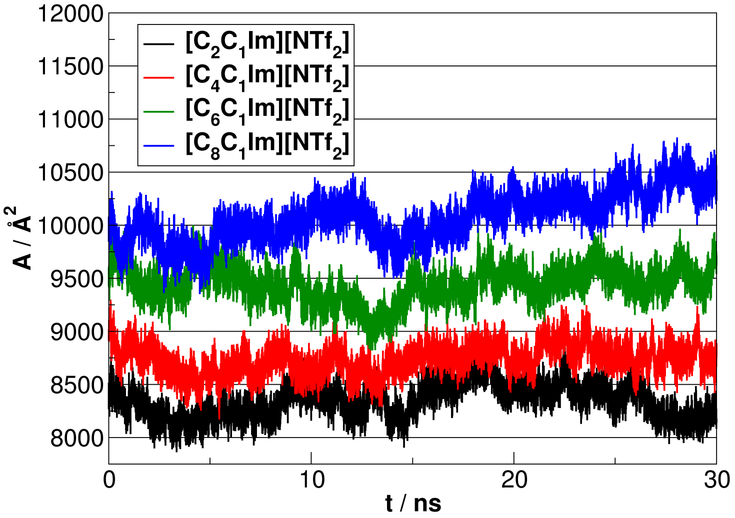

Figure 1: Changes in the surface area A of the PNP versus simulation time in NTf$_2$ ionic liquids, starting from the globular polyethylene PNP.

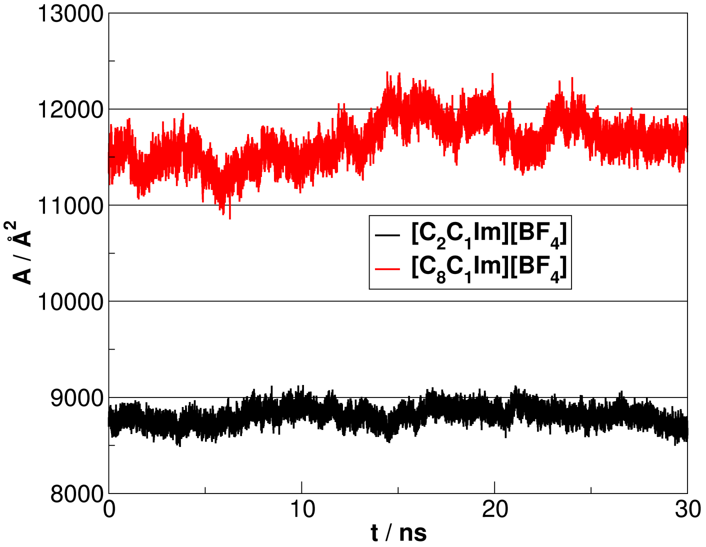

Figure 2: Changes in the surface area A of the PNP versus simulation time in BF$_4$ ionic liquids, starting from the globular polyethylene PNP.

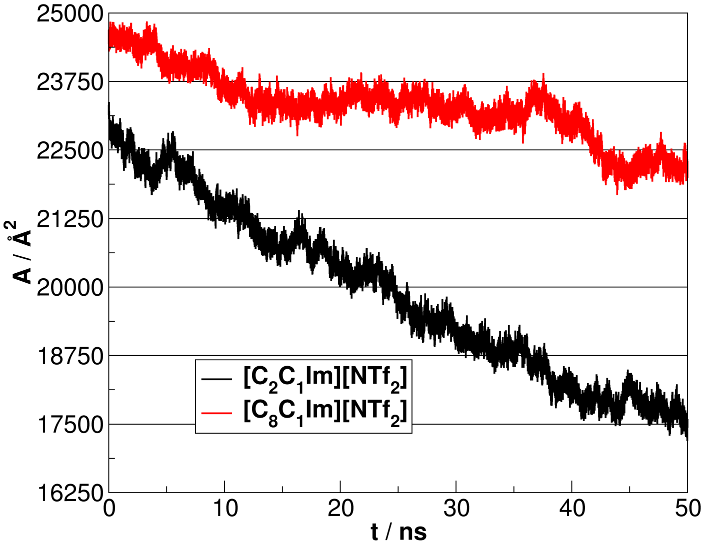

Figure 3: Changes in the surface area A of the PNP versus simulation time in NTf$_2$ ionic liquids, starting from the randomly distributed, dissociated chains.

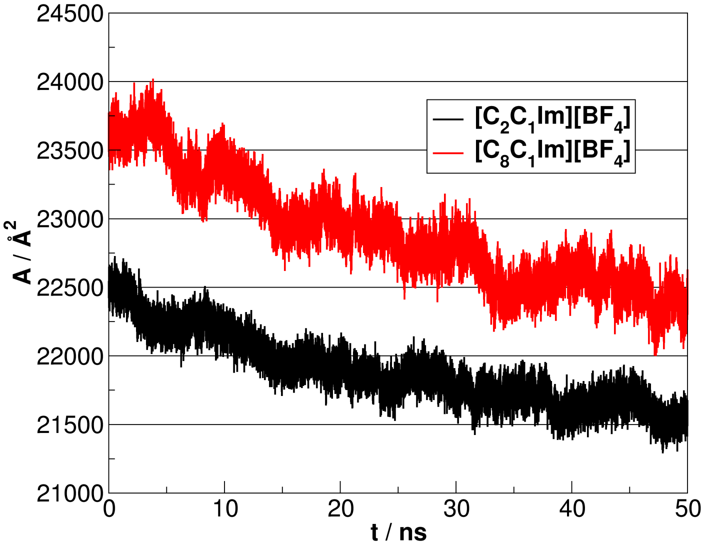

Figure 4: Changes in the surface area A of the PNP versus simulation time in BF$_4$ ionic liquids, starting from the randomly distributed, dissociated chains.

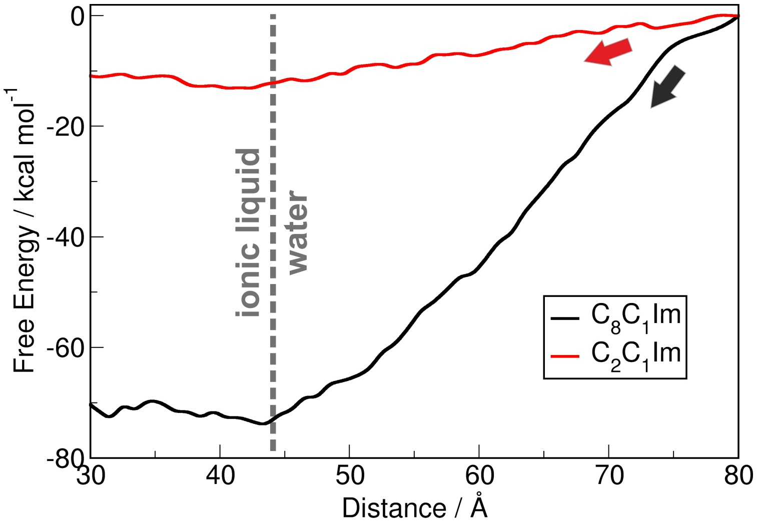

Figure 5: Free energy curves of the phase transfer of the PNP particle from the aqueous phase (right) to the ionic liquid phase (left), obtained from umbrella sampling simulations. The particle was initially situated in the aqueous phase, and gradually moved toward the center of mass of the ionic liquid phase, across the liquid-liquid interface. The location of the particle is defined by the Z component of the distance vector connecting the center of mass of the plastic and that of the ionic liquid phase. The particle crosses the interface at a distance of ca. 44 Å.