A molecular dynamics study on extraction of cations from an ionic liquid droplet under electric field

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Molecular dynamics (MD) simulations have been conducted to investigate the electrophoretic motion of cations and anions in ionic liquid droplets. Recently, interesting retreating behavior of a charged ionic liquid droplet with bis-(trifluoromethylsulfonyl) imide (NTf2) anion in a dielectric liquid medium under electric field has been reported. Experimental studies were performed to verify that the cation extraction phenomenon causes the retreating motion of the ionic liquid droplet. To understand the cation extraction phenomenon clearly through a direct approach to intermolecular interaction between cations and anions, the behavior of ionic liquid droplets under electric field has been investigated with MD simulation in this work. The electrophoretic motions of ionic liquid droplet with NTf2 anion is compared with those of ionic liquid droplet with ethylsulfate (ES) anion to clarify the different molecular behavior of the ions according to the molecular structure of anions. In order to corroborate the cation extraction is affected by intermolecular interaction between cations and anions, intermolecular forces between cations and anions are also discussed.