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A Molecular Dynamics Study on Selective Cation Depletion from an Ionic Liquid Droplet under an Electric Field[1] YUDONG YANG, MYUNGMO AHN, Department of Chemical Engineering, POSTECH, DOJIN IM, Pukyong National University, JUNGMIN OH, Center for Soft and Living Matter, Institute for Basic Science (IBS), INSEOK KANG, Department of Chemical Engineering, POSTECH — General electrohydrodynamic behavior of ionic liquid droplets under an electric field is investigated using MD simulations. Especially, a unique behavior of ion depletion of an ionic liquid droplet under a uniform electric field is studied. Shape deformation due to electric stress and ion distributions inside the droplet are calculated to understand the ionic motion of imidazolium-based ionic liquid droplets with 200 ion pairs of 2 kinds of ionic liquids: EMIM-NTf2 and EMIM-ES. The intermolecular force between cations and anions can be significantly different due to the nature of the structure and charge distribution of the ions. Together with an analytical interpretation of the conducting droplet in an electric field, the MD simulation successfully explains the mechanism of selective ion depletion of an ionic liquid droplet in an electric field. The selective ion depletion phenomenon has been adopted to explain the experimentally observed retreating motion of a droplet in a uniform electric field. The effect of anions on the cation depletion phenomenon can be accounted for from a direct approach to the intermolecular interaction.

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