Electronic Supplementary Material (ESM)

Simulations of structure and dynamics of nanoparticle-based ionic liquids

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Contents

S.1 Movies

I. Ion diffusive behavior in NIMs-L

Filename: "mov_NIMs-L_zoom.avi"

Legend: Video of the diffusive behavior of positive ions of the second generation NIMs with primary amine. Only the ions (negative: blue, positive: red) of a nanoparticle and its neighboring nanoparticles are visible for clarity. The total time corresponding to the video is 36 ns.

Keywords: ionic liquid, nanoparticle.

II. Ion diffusive behavior in NIMs-S

Filename: "mov_NIMs-S_zoom.avi"

Legend: Video of the diffusive behavior of positive ions (red) of third generation NIMs with tertiary amine. Only the ions (negative: blue, positive: red) of a nanoparticle and its neighboring nanoparticles are visible for clarity. The total time corresponding to the video is 36 ns.

Keywords: ionic liquid, nanoparticle.

III. Chain conformation in NIMs-L

Filename: "mov_NIMs-L_chains.avi"

Legend: Video displaying chain conformations and motions of third generation NIMs with primary amine. Only the nanoparticles and the tertiary amines closest to one nanoparticle are visible for clarity. The total time corresponding to the video is 86 ns.

Keywords: ionic liquid, nanoparticle.

IV) Chain conformation in NIMs-S

Filename: "mov_NIMs-S_chains.avi"

Legend: Video displaying the conformations and kinetics of second generation NIMs with tertiary amine. Only the nanoparticles and the tertiary amines closest to one nanoparticle are visible for clarity. The total time corresponding to the video is 86 ns.

Keywords: ionic, liquid, nanoparticle.

V) Nanoparticle diffusive behavior in NOHMs

Filename: "mov_NOHMs_cores.avi"

Legend: Video displaying the nanoparticle diffusive behavior in a NOHM system. Only the nanoparticles are visible for clarity. The total time corresponding to the video is 660 ns.

Keywords: diffusion, ionic liquid, nanoparticle.