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Relaxation dynamics in pyrrolidinium based ionic liquids: the role of the anion conformers.

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Abstract

We report density functional theory (DFT) calculations and low-frequency mechanical spectroscopy results on two ionic liquids having the same *N*-butyl-*N*-methyl-pyrrolidinium cation (PYR₁₄), but different anions, (nonafluorobutanesulfonyl)(toluenesulfonyl)imide (IM_{T4}) and 1,3 hexafluoropropane-disulfonylimide (IM₃), belonging to the per(fluoroalkylsulfonyl)imide family. For both samples, a relaxation process is observed in their supercooled liquid phase, which can be described by a hopping model between non-equivalent configurations. In agreement with previous results, the relaxation is attributed to the ions motion. The comparison among calculations of the anion conformers population and the analysis of the experimental data points out that the

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