Abstract Submitted
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A simulation study of poly(ethylene glycol) in ionic liquids using a physically motivated ab initio force-field[1] EUNSONG CHOI, JESSE G. MCDANIEL, J.R. SCHMIDT, ARUN YETHIRAJ, University of Wisconsin-Madison — The behavior of poly(ethylene glycol) (PEG) in imidazolium-based ionic liquids (ILs) is studied from molecular dynamics simulations using a new physically motivated force-field. The new force-field accounts for various fundamental intermolecular interactions such as electrostatics, induction, exchange, and dispersion in separate terms where the parameters are derived from ab initio, symmetry adapted perturbation theory (SAPT). The crucial point about the new force-field when compared to other existing force-fields is that it is developed free from empirical parameterization; this is a great advantage particularly for the systems like polymer/IL solutions where experimental data are scarce. We first validate the force-field for neat ILs and neat PEG. Then the force-field is applied to the mixture of the two and the final results are compared with available experiments and simulation results using the OPLS-AA force-field.

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