

Abstract Submitted
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Molecular Dynamics Simulations of Liquid, Gel and Polymer Electrolytes OLEG BORODIN, GRANT SMITH, University of Utah — Molecular dynamics simulations have been performed on PEO-based comb-branched polymer electrolytes and liquid electrolytes (ethylene carbonate, propylene carbonate, dimethyl carbonate, oligoethers) doped with LiTFSI and dry and gel single ion conductors with TFSI anions affixed to side chains. Development of the quantum chemistry-based polarizable force field will be discussed. Structural, thermodynamic and transport properties of pure solvents and electrolytes were found in good agreement with experimental data. Transport mechanism, structural and dynamic properties of dry, gel and liquid electrolytes will be discussed.

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