

Abstract Submitted
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Interactions in Ion-containing Polymers Probed by ab initio Methods WENJUAN LIU, RALPH COLBY, Materials Science and Engineering Department, The Pennsylvania State University, MICHAEL JANIK, Department of Chemical Engineering, The Pennsylvania State University, THE PENNSYLVANIA STATE UNIVERSITY TEAM — We use ab initio methods to estimate dipole moments and interaction energetics in ion-containing polymers. Our calculation quantitatively includes electrostatic interactions (using both permanent and induced dipoles) and effectively estimates solvation energetics for ions interacting with various functional groups. Interactions are reported for various small cations with common functional groups on polymers and carboxylate, sulfonate and phosphate groups that can be present in anionic ionomers. We demonstrate how these interaction energies can be utilized to design polymer membranes with facile ion transport.

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