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Ionomer Design, Synthesis and Characterization for Ion-Conducting Energy Materials[1]

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For ionic actuators and battery separators, it is vital to utilize single-ion conductors that avoid the detrimental polarization of other ions; the commonly studied dual-ion conductors simply will not be used in the next generation of materials for these applications. *Ab initio* quantum chemistry calculations at 0 K in vacuum characterize ion interactions and ion solvation by various functional groups, allowing identification of constituents with weak interactions to be incorporated in ionomers for facile ion transport. Simple ideas for estimating the ion interactions and solvation at practical temperatures and dielectric constants are presented that indicate the rank ordering observed at 0 K in vacuum should be preserved. Hence, such *ab initio* calculations are useful for screening the plethora of combinations of polymer-ion, counterion and polar functional groups, to decide which are worthy of synthesis for new ionomers. Single-ion conducting ionomers are synthesized based on these calculations, with low glass transition temperatures (facile dynamics) to prepare ion-conducting membranes for ionic actuators and battery separators. Characterization by X-ray scattering, dielectric spectroscopy, NMR and linear viscoelasticity collectively develop a coherent picture of ionic aggregation and both counterion and polymer dynamics. Examples are shown of how *ab initio* calculations can be used to understand experimental observations of dielectric constant, glass transition temperature and conductivity of polymerized ionic liquids with counterions being either lithium, sodium, fluoride, hydroxide (for batteries) or bulky ionic liquids (for ionic actuators).

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