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Quantum mechanical calculation of ion chains in Poly(ethylene oxide)-based Sulfonate Ionomers[1] HUAI-SUEN SHIAU, MICHAEL JANIK, RALPH COLBY, Pennsylvania State University, DOE LI+ BATTERY ENERGY PROJECT TEAM — Ion-containing polymers are of interest as single-ion conductors for use as electrolytes in electrochemical devices, including lithium ion batteries. Current ion conductivities of the best ionomers are roughly 100X too small for practical applications and have a small fraction of their Li^+ counterions participating in conduction. *Ab initio* methods are used to investigate the dissociation/association of ionic chain aggregates. The binding energy as a function of distance between ions is explored, in which the energy at each separation is optimized with respect to the number and location of solvating ether oxygen moieties. We study the barrier between the solvated and bound states as a function of distance between the ions, including the barrier to break ion chain aggregates in different positions along the chain. This is prerequisite to mesoscale simulations capable of reproducing the equilibrium between various ion chain aggregates, with realistic dynamics, from which conductivity pathways can be investigated.

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