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Simulation of a Small Molecule Analogue of a Lithium Ionomer in an External Electric Field JOHN MCCOY, New Mexico Tech, SARA WATERS, Applied Sciences Laboratory, Washingtion State Univ., AMALIE FRISCHKNECHT, Sandia National Laboratories, JONATHAN BROWN, Ohio State Univ. — Ion dynamics were studied in lithium-neutralized 2-pentylheptanoic acid, a small molecule analogue of a precise poly(ethylene-co-acrylic acid) lithium ionomer. Atomistic molecular dynamics simulations were performed in an external electric field. The electric field causes alignment of the ionic aggregates along the field direction. The energetic response of the system to an imposed oscillating electric field for a wide range of frequencies was tracked by monitoring the coulombic contribution to the energy. The susceptibility found in this manner is a component of the dielectric susceptibility typically measured experimentally. A dynamic transition is found and the frequency associated with this transition varies with temperature in an Arrhenius manner. The transition is observed to be associated with rearrangements of the ionic aggregates.

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