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Molecular Dynamics Simulation of Diffusivity and Mobility of Ionic Charge Carriers in Model Battery Polymers SARA WATERS, JON BROWN, New Mexico Institute of Mining and Technology, AMALIE FRISCHKNECHT, Sandia National Labs, JOHN MCCOY, New Mexico Institute of Mining and Technology — Molecular dynamics simulations of poly(ethylene-co-acrylic acid) monomers doped with Lithium ions were conducted using LAMMPS. The drift velocity of the ions resulting from a range of static electric fields were used to compute the ionic mobility. The frequency dependent mobility was also studied by using oscillatory electric fields.

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