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Ion Diffusion in Battery Materials Probed with βNMR and μSR

IAIN MCKENZIE, TRIUMF, DAVID CORTIE, The Australian National Univ., STEPHEN COTTRELL, ISIS, Rutherford Appleton Lab., MASASHI HARADA, Toyota Central Research and Development Lab., Inc., ROBERT KIEFL, Univ., of British Columbia, PHILIP LEVY, TRIUMF, ANDREW MACFARLANE, RYAN MCFADDEN, Univ., of British Columbia, GERALD MORRIS, TRIUMF, SHIN-ICHI OGATA, Toyota Central Research and Development Lab., Inc., MATTHEW PEARSON, TRIUMF, JUN SUGIYAMA, Toyota Central Research and Development Lab., Inc. — Radioactive beam magnetic resonance techniques, β-detected NMR (β-NMR) and muon spin rotation and relaxation (μSR), have been used to study the microscopic diffusion of lithium ions and muons (Mu^+), which can be considered light protons, in poly(ethylene oxide) (PEO), a common polymer electrolyte in lithium ion batteries. β-NMR measurements were performed on thin films of PEO with lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) and lithium trifluoroacetate (LiTFA) with monomer-to-salt ratios of 8.3. Hopping of $^8\mathrm{Li}^+$ above $\sim$250 K follows an Arrhenius law in all of the films. The diffusion parameters of $^8\mathrm{Li}^+$ in the salt-containing films are strongly correlated with the ionicity of the lithium salt rather than the glass transition temperature of the sample. The intrinsic hop rate increases exponentially with ionicity, while the activation energy for hopping increases approximately linearly going from 6.3 ± 0.2 kJ/mol in PEO:LiTFA to 17.8 ± 0.2 kJ/mol in PEO:LiTFSI. $^8\mathrm{Li}^+$ diffusion is fastest in pure PEO. Hopping of Mu^+ is observed in pure PEO above the glass transition temperature with an activation barrier of 11.8 ± 0.1 kJ/mol.

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