Abstract Submitted
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Diffusion of lithium ions in amorphous and crystalline PEO_3:$LiCF_3SO_3$ polymer electrolytes: ab initio calculations and simulations[1] SHA XUE, YINGDI LIU, YAPING LI, DALE TEETERS, DANIEL CRUNKLETON, SANWU WANG, The University of Tulsa — The PEO_3:$LiCF_3SO_3$polymer electrolyte has attracted significant research due to its high conductivity and enhanced stability in lithium polymer batteries. Most experimental studies have shown that amorphous PEO lithium salt electrolytes have higher conductivity than the crystalline ones. Other studies, however, have shown that crystalline phase can conduct ions. In this work, we use ab initio molecular dynamics simulations to obtain the amorphous structure of PEO_3:$LiCF_3SO_3$. The diffusion pathways and activation energies of lithium ions in both crystalline and amorphous PEO_3:$LiCF_3SO_3$are determined with first-principles density functional theory. In crystalline PEO_3:$LiCF_3SO_3$, the activation energy for the low-barrier diffusion pathway is approximately 1.0 eV. In the amorphous phase, the value is 0.6 eV. This result would support the experimental observation that amorphous PEO_3:$LiCF_3SO_3$has higher ionic conductivity than the crystalline phase.

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