

Abstract Submitted  
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**Molecular dynamics simulation of low dielectric constant polymer electrolytes**<sup>1</sup> BILL WHEATLE, NATHANIEL LYND, VENKAT GANESAN, Univ of Texas, Austin — Recent experimental studies measured the ionic conductivities of a series of poly(glycidyl ether)s with varying neat dielectric constants ( $\epsilon$ ), viscosities ( $\eta$ ), and glass transition temperatures ( $T_g$ ), as hosts for lithium bistrifluoromethanesulfonimide (LiTFSI) salt. In such a context, it was demonstrated that the ionic conductivity of these polymer electrolytes was a function of  $\epsilon$  rather than  $T_g$  or  $\eta$ , suggesting that there may exist regimes in which ionic conductivity is not limited by slow segmental dynamics but rather by low ionic dissociation. Motivated by such results, we used atomistic molecular dynamics to study the structure and transport characteristics of the same set of host polymers. We found that the coordination number of TFSI<sup>-</sup> about Li<sup>+</sup> in the first solvation shell and the total fraction of free ions increased as a function of  $\epsilon$ , implying the polymer hosts enhanced ion dissociation. In addition, we found that increasing the dielectric constant of the host polymer enhanced self-correlated ion transport, as evidenced by an increase in the diffusion coefficients of each ion species. Overall, we confirmed that limited ion dissociation in low- $\epsilon$  polymer electrolyte hosts hampers ionic conductivity.

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