

Abstract Submitted  
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**Effects of Structured Ionomer Interfaces on Water Diffusion: Molecular Dynamics Simulation Insight**<sup>1</sup> DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY GREEST, Sandia National Laboratory — The dynamics of solvent molecules across structured ionomers interfaces is crucial to innovative technologies with selective controlled transport. These polymers consist of ionizable blocks facilitating transport tethered to mechanical stability enhancing ones, where their incompatibility drives compounded interfaces. Here water penetration through the interface of an A-B-C-B-A co-polymer is probed by atomistic molecular dynamics simulations where C is a randomly sulfonated polystyrene with sulfonation fractions  $f = 0$  to 0.55, B is poly (ethylene-r-propylene) and A is poly (t-butyl styrene). For  $f > 0$ , a two-step process with slow diffusion at the early stages is observed where water molecules transverse the hydrophobic rich surface before reaching the hydrophilic regime. Water molecules then diffuse along the percolating network of the ionic center block. Increasing the temperature and sulfonation fraction enhances both the rate of diffusion and the overall water uptake.

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