

Abstract Submitted
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Molecular-dynamics study of proton transport near an ionomer-electrode interface¹ PHILIP TAYLOR, ELSHAD ALLAHYAROV, Case Western Reserve University — Coarse-grained molecular-dynamics simulations have been used to study the behavior of an ionomer electrolyte in response to an induced current. We observe the changes in the distribution of charge concentration and local electrostatic field in the region near an electrode in contact with a Nafion-like ionomer. We have also analyzed how the morphology of the sulfonate clusters and the transport of water molecules depends on the current strength. In this study we insert protons at the electrode interface of the material and remove them at a plane some distance into the material. When a steady state is achieved we note the new charge distribution and average voltage difference between the faces of the simulation cell. We also note the change in distribution of water molecules within the material in response to the induced current of protons. We compare these results with those predicted by one-dimensional theoretical models.

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