

Abstract Submitted
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Simulation study of charge distribution near an ionomer-electrode interface¹ ELSHAD ALLAHYAROV², PHILIP TAYLOR, Physics Department, Case Western Reserve University, Cleveland OH, USA — Molecular dynamics simulations have been used to investigate the nature of the electrostatic field and of the proton density distribution in a Nafion-like ionomer in contact with an electrode. We compare our results for a heterogeneous ionomer, in which a partial phase separation has resulted in separate nanoscopic regions of hydrophobic and hydrophilic material, with those predicted by one-dimensional theoretical models in which Poisson-Boltzmann techniques are used to derive self-consistent potentials and concentration distributions. We further examine the effects of the strong inhomogeneous electrostatic fields in changing the morphology of the ionomer in the vicinity of the electrode from its original form in the bulk material.

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