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Simulation study of proton transport in a cylindrically confined ionomer channel[1] ELSHAD ALLAHYAROV, PHILIP TAYLOR, Case Western Reserve University, HARTMUT LÖWEN, Heinrich-Heine University Dusseldorf, Germany — Coarse-grained simulation methods have been used to investigate confinement-induced morphological changes in Nafion-like ionomers and their effect on proton conductivity. The system we study models a cylindrical pore in a matrix of supporting material that can be hydrophilic or hydrophobic, with pore diameters that vary from 2 to 7 nm. We report results that indicate the dependence of the equilibrium structure on the matrix material and pore diameter, and on the humidity of the ionomer as defined by the ratio, λ, of the number of water molecules to the number of sulfonate groups. In particular, we report the relationship between cylinder diameter and the existence of continuous pathways for proton conductance at low levels of humidity. These suggest an optimum diameter and hydrophobicity for fuel-cell membranes composed of an impervious matrix penetrated by cylindrical ionomer-filled pores.

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