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Simulation study of proton transport in stretched nanocomposite ionomer fuel-cell membranes[1] PHILIP TAYLOR, ELSHAD ALLAHYAROV, Case Western Reserve University — We have used coarse-grained simulation methods to investigate the effect of inclusions of nanoparticles on the stretching-induced structure orientation and on the proton conductivity of polymer electrolyte membranes. Uniaxial stretching of a Nafion film containing no inclusions causes a modest increase in proton conductivity in the direction of stretching. This effect does not persist to any significant degree after removal of the stretching stress. Stretching of a Nafion film containing spherical nanoparticles, on the other hand, causes a large increase in proton conductivity in the direction of stretching, and this effect persists to a much greater extent after the removal of the stretching stress. Simulations were performed with monodisperse nanoparticles whose diameters were in the range from 17 to 28 nm, and whose surfaces were either hydrophilic, neutral, or hydrophobic. The greatest effect in causing enhancement of the proton conductivity and in causing persistent ordering was found for hydrophilic nanoparticle inclusions of 28 nm diameter.

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