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The role of nanoparticle-membrane coupling in nanocomposite ionomers[1] ELSHAD ALLAHYAROV, PHILIP TAYLOR, Case Western Reserve University — Coarse-grained simulation methods have been used to investigate the effect of inclusions of spherical nanoparticles on the properties of Nafion®-like membranes. We find the clustering of the sulfonate head groups to be strongly affected by the presence of a monodisperse array of spheres when the sphere diameters lie in the range from 17 to 28 nm. This change in morphology enhances the proton conductivity of the membrane through the formation of channels connecting adjacent clusters. This effect was characterized in terms of the distribution of channel lengths of the hydrophilic phase. Simulations were performed for Nafion containing spherical nanoparticles whose surfaces were either hydrophilic, neutral (hard core), or hydrophobic. The diameters of the nanoparticles were changed while keeping fixed the volume fraction of inclusions. We find that the proton conductivity of these nanocomposites is always higher than the conductivity of ionomers without additives. This effect becomes most pronounced in nanocomposites containing particles whose surfaces are hydrophilic, and whose diameters are in the larger part of the range of sizes examined.

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