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Weak polyelectrolytes in Confined Geometries JONATHAN K. WHITMER, VIKRAMJIT S. RATHEE, BENJAMIN SIKORA, University of Notre Dame — Crucial to the behavior of recently designed charge-rejection and mosaic membranes are the conformations of polyelectrolyte brushes and oligomeric grafts used to control the membranes' surface charge. The use of pH-tunable weak polyelectrolytes with associative interactions enables fine tuning of material transport properties. Here, we apply constant-pH molecular dynamics along with free energy sampling algorithms to understand the subtle tug-of-war between pH, salt concentrations, and solvation forces in confined systems, and determine how each of these effects alters transport within the system. We further discuss the implications of our findings for the design of electrolyte separation membranes.

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