

Abstract Submitted  
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**Thermodynamics of Ionic Transport through Functionalized Membranes** VIKRAMJIT RATHEE, SIYI QU, THEODORE DILENSCHNEIDER, WILLIAM A. PHILLIP, JONATHAN K. WHITMER, Chemical and Biomolecular Engineering, University of Notre Dame — Through microphase separation of block copolymers, highly porous solid membranes may be assembled. Further functionalization with amine and sulfonic acid groups has demonstrated promise in exquisitely controlling the flux of charged species, and in particular multivalent ions. Using coarse-grained molecular simulations, we explore the essential thermodynamics underlying salt rejection in charge-functionalized membranes, and develop a model capable of linking the performance of these membranes to their molecular character through free energy calculations.

Vikramjit Rathee  
Univ of Notre Dame

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