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Molecular Simulation Evaluation of Macromolecular Transport through Nanofiltration Membranes NOELIA ALMODOVAR ARBELO, BRYAN BOUDOURIS, DAVID CORTI, Purdue University — A hybrid Monte Carlo and Molecular Dynamics simulation technique was implemented to elucidate the equilibrium behavior and transport properties of a model macromolecule as it navigated across a nanoporous polymer thin film (i.e., a nanofiltration membrane). The model linear homopolymer chosen was one that had interactions that were representative of poly(ethylene oxide) (PEO) due to the known interactions of PEO with solution molecules when a PEO chain is dissolved in an aqueous environment. The structural rearrangements of the PEO chain as it passes through the nanopore under an imposed chemical potential gradient was quantified as a function of solvent quality, polymer chain length, nanopore diameter and shape, and PEO-nanopore wall interactions. Thus, these computational studies provide a more detailed picture of the underlying physical mechanisms that drive macromolecular transport through nanopores, and, in particular, how dimensionally-large macromolecules (i.e., with large radii of gyration) enter and move through dimensionally-small pores (i.e., small radii nanopores). The insights gained from these studies will aid in the development of more cost-effective water purification systems in separation technologies for myriad industrial applications.

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