Seeing the Invisible: Molecular Simulations Redefining Membrane Operations

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Membrane processes are increasingly challenged to achieve higher separation efficiency under stringent energy and material constraints. Transport phenomena govern their performance at nanoscales and at dynamic interfaces, where molecular interactions within confined environments remain largely inaccessible to experimental observation. Molecular simulations provide a unique framework for accessing these scales, enabling direct analysis of transport pathways, interfacial phenomena, and dynamic molecular rearrangements that determine separation performance. Beyond their traditional interpretative role, simulations are increasingly enabling the quantification of mechanisms governing selectivity, transport anomalies, and interfacial processes such as nucleation and crystallization at membrane surfaces. When integrated with experimental studies, multiscale modeling, and machine learning approaches, molecular simulations establish quantitative links between molecular behavior and macroscopic process performance. This integration is driving a transition from empirically optimized systems to predictive, rationally designed membrane processes. In this perspective, molecular-level phenomena are no longer hidden variables but become actionable parameters for process design, opening new opportunities for the development of more efficient and sustainable separation technologies. When combined with experimental studies, multiscale modeling, and machine learning, molecular simulations enable the transition from empirically optimized systems to rationally designed, predictive membrane processes. Seeing the invisible is therefore not only a matter of understanding, but a prerequisite for predictive membrane process design.