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Microscopic Insights into Water Transport Through a Biomimetic Artificial Water Nano-Channels-Polyamide Membrane

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Abstract : Clean water is ubiquitous from drinking to agriculture and from energy supply to industrial manufacturing. Since the conventional water sources are becoming increasingly rare, the development of new technologies for water supply is crucial to address the world's clean water needs in the 21st century. Desalination is in many regards the most promising approach to long-term water supply since it potentially delivers an unlimited source of fresh water. Seawater desalination using reverse osmosis (RO) membranes has become over the past decade a standard approach to produce fresh water. While this technology has proven to be efficient, it remains however relatively costly in terms of energy input due to the use of high-pressure pumps resulting of the low water permeation through polymeric RO membranes. Recently, water channels incorporated in lipidic and polymeric membranes were demonstrated to provide a selective water translocation that enables to break permeability- selectivity trade-off. Biomimetic Artificial Water channels (AWCs) are becoming highly attractive systems to achieve a selective transport of water. The first developed AWCs formed from imidazole quartet (I-quartet) embedded in lipidic membranes exhibited an ion selectivity higher than AQPs however associated with a lower water flow performance. Recently it has been conducted pioneer work in this field with the fabrication of the first AWC@Polyamide(PA) composite membrane with outstanding desalination performance. However, the microscopic desalination mechanism in play is still unknown and its understanding represents the shortest way for a long-term conception and design of AWC@PA composite membranes with better performance. In this work we gain an unprecedented fundamental understanding and rationalization of the nanostructuration of the AWC@PA membranes and the microscopic mechanism at the origin of their water transport performance from advanced molecular simulations. Using osmotic molecular dynamics simulations and a non-equilibrium method with water slab control, we demonstrate an increase in porosity near the AWC@PA interfaces, enhancing water transport without compromising the rejection rate. Indeed, the water transport pathways exhibit a single-file structure connected by hydrogen bonds. Finally, by comparing AWC@PA and PA membranes, we show that the difference in water flux aligns well with experimental results, validating the model used.

Keywords : water desalination, biomimetic membranes, molecular simulation, nanochannels
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