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Introduction to molecular engineering for water technologies

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Challenges are mounting globally with respect to both water quality and quantity, driven by unsustainable practices, aging infrastructure, climate change, urbanization, and other macrotrends. This collection presents recent studies such as material design for nanofiltration, electrodeionization, and water monitoring; experimental and computational studies of transport through membranes; and modeling of bulk water by using sparse training data sets. Research progress on membranes and solar evaporators is also reviewed from the perspective of molecular engineering.

Membrane technologies have been widely applied in desalination and wastewater treatment. Molecular engineering of membrane materials is highlighted in the article by Phillip *et al.* (DOI: 10.1039/C9ME00160C) and the mini-review by Yang, Darling *et al.* (DOI: 10.1039/C9ME00154A). Phillip *et al.* develop a hollow fiber nanofiltration membrane from the microphase separation of a designed copolymer followed by cross-linking. The membrane with nanopores delivers both high flux and rejection of divalent cations after surface functionalization with positively charged moieties, presenting a good example of how molecular and interfacial engineering can impart tailored separation performance. The mini-review by Yang, Darling and co-workers summarizes the

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Seth B. Darling

Seth B. Darling is the Director of the Center for Molecular Engineering and a Senior Scientist in the Chemical Sciences & Engineering Division at Argonne National Laboratory. He also serves as the Director of the Advanced Materials for Energy-Water Systems (AMEWS) Energy Frontier Research Center. He received his PhD in physical chemistry from the University of Chicago. His group's research centers around molecular engineering with a current emphasis on advanced materials for cleaning water, having made previous contributions in fields ranging from self-assembly to advanced lithography to solar energy. He has published over 125 scientific articles, holds a dozen patents, is a co-author of popular books on water and on debunking climate skeptic myths, and lectures widely on topics related to energy, water, and climate.

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most recent progress in molecular engineering on organic–inorganic composite membranes with different configurations. Molecular engineering of the organic–inorganic interface can enhance interface compatibility and promote membrane performance in separation and purification processes.

Solar steam generation by an interfacial photothermal evaporator is an emerging technique to acquire freshwater from brine or to concentrate wastewater. Cao and co-workers (DOI: 10.1039/C9ME00166B) highlight the appealing applications of solar-driven evaporators from the view of structure design. Both molecular architecture and macro-structure design can promote the photothermal efficiency of these systems.

Electrodeionization (EDI) is another promising separation process for water purification—particularly in applications of moderate salinity or where selective ion separation or recovery is desirable. To further improve the energy efficiency, Lin, Arges *et al.* (DOI: 10.1039/C9ME00179D) develop a Janus bipolar resin wafer incorporated with a water dissociation catalyst, $Al(OH)_3$ nanoparticles, to promote water-splitting. The Janus bipolar resin wafers can augment the diluate chamber ionic conductivity in EDI setups and overcome the limitations of large electrolyte feed concentration requirements in conventional biopolar membrane electrodialysis.

Any treatment strategy will hinge on knowledge of the feed water chemistry. Sensitive detection of harmful ions in water, for example, is important for residential water security, and enriched phosphate or other nutrient ions in waterways may lead to eutrophication. Chen *et al.* (DOI: 10.1039/C9ME00156E) demonstrate a real-time phosphate ion sensor based on ferritin probes with ultra-high sensitivity. Reduced graphene oxide nanosheets serve as the sensing channels, followed by the atomic layer deposition of Al_2O_3 as a passivation layer to separate the sensing channels from the sample solution. The sensor achieves a lower detection limit of 10 μg L^{-1}.

Water systems are remarkably complex, and often it is essential to apply theory, modelling, and simulation methods to interpret or guide experimental efforts. Molecular dynamics simulation, in particular, is a powerful tool to reveal the molecular-to-microscale evolution of material systems. Sankaranarayanan and co-workers (DOI: 10.1039/C9ME00184K) present an active learning approach that can achieve accurate force-fields by using extremely sparse training data sets. They train a neural network to reproduce thermodynamic, structural, and transport properties of bulk liquid water by sampling fewer than 300 configurations and their energies, which hints at tremendous promise in a range of other systems.

Coupling modelling and experiment, Hassanali, Chiavazzo *et al.* (DOI: 10.1039/C9ME00186G) present interesting work on gas transport through soap-film membranes, a special aqueous system. Their molecular model is validated against experimental data from purposely designed experiments. The results reveal that CO_2 tends to get trapped within the hydrophobic tail of the surfactant molecules.

We acknowledge the valuable contributions from all the authors in this themed collection and hope that readers will draw inspiration from these articles and continue to push the frontiers of molecular engineering for water.