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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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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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Hao-Cheng Yang is an Associate Professor in the School of Chemical Engineering at Sun Yat-Sen University. He received his B.E. degree in polymer materials and engineering from Zhejiang University in 2012, and received his Ph.D. degree in polymer science from the same university in 2017. He then joined Dr. Darling's group at Argonne National Laboratory as a postdoctoral researcher and became an Associate Professor at

Sun Yat-Sen University in 2018. His group focuses on the surface and interface engineering of macroscopic two-dimensional materials such as separation membranes, functional coatings and films. He has published over 60 scientific papers on the topic of membrane science and technology.

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, $\text{Al}(\text{OH})_3$ 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 bipolar 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 $10\ \mu\text{g L}^{-1}$.

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.