

## Computational Materials Discovery for Reverse Osmosis Desalination and Water Harvesting

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Water scarcity has become one of the most difficult challenges of our time. Producing clean water from unconventional sources is therefore of utmost importance. Specifically, desalinating saline water via reverse osmosis (RO) membrane processes (i.e., RO desalination) and harvesting atmospheric water via adsorption (i.e., water harvesting) represent promising approaches. To enable more cost-effective and energy-efficient processes for clean water production, discovering novel RO membranes and optimal water adsorbents is critical. Computational studies can play an important role in such development to identify promising candidates with atomic-level understandings. This presentation will discuss our recent efforts, by employing molecular simulations including both molecular dynamics and Monte Carlo calculations, to unravel the design of nanoporous materials for these two applications. Our recent development of more efficient simulation approaches to determine water adsorption properties in porous materials will also be introduced.