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Optimizing Nanopore Surface Properties for High-Efficiency Water Desalination DAVID COHEN-TANUGI, JEFFREY GROSSMAN, Massachusetts Institute of Technology — As water resources worldwide become rapidly scarcer, it is becoming increasingly important to devise new techniques to obtain clean water from seawater. At present, water purification technologies are limited by costly energy requirements relative to the theoretical thermodynamic limit and by insufficient understanding of the physical processes underlying ion filtration and fluid transport at the molecular scale. New advances in computational materials science offer a promising way to deepen our understanding of these physical phenomena. In this presentation, we describe a new approach for high-efficiency water desalination based on surface-engineered porous materials. This approach is especially relevant for promising technologies such as nanofiltration and membrane distillation, which offers promising advantages over traditional desalination technologies using mesoporous membranes that are only permeable to pure water vapor. More accurate molecular modeling of mesoporous and nanoporous materials represents a key step towards efficient large-scale treatment of seawater. Results regarding the effect of pore properties (surface texture, morphology, density, tortuosity) on desired performance characteristics such as ion selectivity, maximal water flux and energy requirements will be presented.

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