Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Computational nanomaterials for novel desalination membrane design: Nanoporous graphene DAVID COHEN-TANUGI, MIT, JEFFREY C. GROSSMAN, Department of Materials Science & Engineering, MIT — We describe a novel approach for desalination based on nanoporous graphene. Our molecular dynamics calculations show that freestanding graphene patterned with nanometer-sized pores can act as an ultra-thin filtration membrane. Due to size exclusion and chemical interactions with the confining pores, salt ions can be blocked from permeating the membrane at sufficiently small pore diameters. Notably, the pore diameter and the chemical interactions at the water-membrane interface are most important criteria for this system's desalination performance. We will share insights from Molecular Dynamics calculations regarding the theoretical performance of this membrane system and the effects of chemical passivation of the graphene pores on the filtration dynamics. Although the narrow range of acceptable pore sizes suggests that further design innovations will be necessary at the molecular scale before large-scale applications are possible, our existing results predict that pressure requirements for this system can be made roughly competitive with commercial Reverse Osmosis.

David Cohen-Tanugi
MIT

Date submitted: 28 Dec 2011 Electronic form version 1.4