Abstract Submitted
for the DFD10 Meeting of
The American Physical Society

Atomistic simulation of water transport through graphene membrane MYUNG EUN SUK, NARAYANA ALURU, University of Illinois — Graphene monolayer can be considered as the thinnest membrane reported so far as its thickness is only one carbon atom diameter. In this study, water transport through porous graphene membrane is investigated using molecular dynamics simulations. Water flux through graphene is compared to the water flux through thin (less than 10 nm in thickness/length) carbon nanotube (CNT) membranes at various diameters. For small diameter, where single-file structure is observed, water flux is lower through the graphene membrane compared to that of the CNT membrane. On the other hand, for larger diameter pores, where the single-file structure is no longer observed, water flux is higher through the graphene membrane, compared to that of the CNT membrane. We explain the results using hydrogen bonding dynamics, pressure distribution and potential of mean force.

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Date submitted: 06 Aug 2010 Electronic form version 1.4