Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Quantized Water Transport: Ideal Desalination through Graphyne-4 Membrane CHONGQIN ZHU, HUI LI, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, XIAO CHENG ZENG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, E.G. WANG, School of Physics and International Center for Quantum Materials, Peking University, SHENG MENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences — The shortage of clean and fresh water is one of most pervasive problems afflicting human being's life in the world. Desalination is one viable solution to produce clean water, since 98% of the available water in the form of salty water. Using molecular dynamics simulations, we demonstrate that graphyne sheet exhibits promising potential for nanoscale desalination to achieve both high water permeability and salt rejection rate. In addition, Graphyne sheets also are mechanically robust with high tolerance to deformation. Especially, γ-graphyne-4 has the best performance with 100% slat rejection and an unprecedented water permeability of $\sim$ 13L/cm2/day/MPa. 3 orders of magnitude higher than prevailing commercial membranes based on reverse osmosis, and $\sim$ 10 times higher than the state-of-the-art nanoporous graphene. Strikingly, water permeability across graphyne exhibits unexpected nonlinear dependence on the pore area. This counter-intuitive behavior is attributed to the quantized nature of water flow at the nanoscale, which has wide implications in controlling nanoscale water transport and designing highly effective membrane.

Chongqin Zhu
Beijing National Laboratory for Condensed Matter Physics,
and Institute of Physics, Chinese Academy of Sciences

Date submitted: 07 Nov 2013 Electronic form version 1.4