Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ion transport and dehydration in sub-nanoscale pores[1] SUBIN SAHU, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899, MASSIMILIANO DI VENTRA, Department of Physics, University of California, San Diego, CA 9500, MICHAEL ZWOLAK, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD — Ions in solution develop tightly bound layers of water – hydration layers – which stabilize disassociation and enable ionic currents to flow. Sub-nanometer pores in a membrane enable ions to pass provided that they shed their hydration shell. This process has an associated large energy penalty that is predicted to give rise to "quantized" steps in the ionic conductance.[2,3] Using all-atom molecular dynamics simulation, we demonstrate that the ionic current begins to show nonlinear behavior as the radius of the pore is reduced to the sub-nanometer scale. This nonlinear behavior is seen as a sharp rise in the pore resistance and excess noise in the current. Our work sheds light on basic mechanism of ion transport through sub-nanoscale pores.

[1]S. Sahu acknowledges support by UMD/CNST Cooperative Research Agreement, Award 70NANB10H193 through University of Maryland
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[3]Zwolak, M., Wilson, J. & Di Ventra, M. Dehydration and ionic conductance quantization in nanopores. *J. Phys.: Condens. Matter* **22**, 454126 (2010).

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Date submitted: 05 Nov 2015 Electronic form version 1.4