

Abstract Submitted
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Probing Water Structures in Nanopores via Tunneling¹ PAUL BOYNTON, MASSIMILIANO DI VENTRA, University of California, San Diego — We study the effects of volumetric constraints on the structure and electronic transport properties of distilled water in a synthetic nanopore. Combining classical molecular dynamics simulations with the Landauer approach to scattering theory as originally done in the context of DNA sequencing [1], we develop a relationship between the electronic current and the structure the water assumes in the confining pore-electrode system. Prior research in the field shows a tendency for the tunneling current through water to fluctuate due to local cavities in the water's structure. We show a shift in the tunneling current's dependence on pore diameter at the transition from exclusion of water to a monolayer. Furthermore, we argue that the current with respect to pore diameter does not follow a simple exponential curve at this transition as one would expect from tunneling. This research develops our understanding of water as a complex medium and describes fundamental physics of aqueous solutions.

[1] J. Lagerqvist, M. Zwolak, and M. Di Ventra, *Fast DNA sequencing via transverse electronic transport*, Nano Lett. **6**, 779 (2006).

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Paul Boynton
University of California, San Diego

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