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Dehydration and Ionic Conductance Quantization in Synthetic Nanopores[1] JAMES WILSON, University of California San Diego, MICHAEL ZWOLAK, MASSIMILIANO DI VENTRA — Synthetic nanopores and nanochannels create new opportunities - beyond biological ion channels - to study ionic transport at the nanoscale. One process that occurs at this scale is dehydration. Ions in water do not move freely, but are instead surrounded by tightly bound water molecules held by the charge-dipole interaction. These water molecules are organized into hydration layers. For the ion to move through a nanopore of sufficiently small radius, these hydration layers must be shed as there is not enough space within the pore to accommodate them. We use molecular dynamics simulations to develop a model of dehydration based on the energy cost associated with removing water molecules. We predict that the ionic current would show sudden drops as the pore radius is reduced due to the exclusion of the hydration layers. We also examine the effect of both the sign and magnitude of the ion charge, demonstrating that divalent ions will more clearly exhibit the effect of dehydration on the ionic current.

[1] M. Zwolak, J. Wilson, and M. Di Ventra, J. Phys.: Condens. Matter 22, 454126 (2010); See also M. Zwolak and M. Di Ventra, Phys. Rev. Lett. 103, 128102 (2009)

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