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**Density Functional Theory calculations of energies of ions in water and in nanopores**[1] KEVIN LEUNG, Sandia National Laboratories, MARTIJN MARSMAN, Universitat Wien — Accurate estimates of ion hydration and electrostatic energies are critical for predicting the permeation or rejection of ions in water-filled nanopores. Ab initio Molecular Dynamics methods (AIMD), based on Density Functional Theory (DFT), accounts for the electronic properties and polarizability of materials, water molecules, and ions, and it may appear to be the method of choice for predicting accurate ion energies in water and in nanopores. In practice, applying DFT coupled with the use of periodic boundary conditions in a charged simulation cell leads to anomalous shifts in the electrostatic potential. Using the projector augmented-wave (PAW) method, Wannier functions, and appropriate corrections, we report energies of ions in several systems that can be referenced to interfaces or unambiguous ("vacuum") values.

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