

Abstract Submitted  
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**Pressure-Actuated Influx and Outflow of Aqueous NaCl in Hydrophobic Nanopores**<sup>1</sup> DUSAN BRATKO, SERBAN GABRIEL ZAMFIR, VCU — Compression of water in hydrophobic pores has been established as a viable mechanism for conversion of mechanical work to interfacial free energy as new form of energy storage or absorption. Reducing the hysteresis of the influx/outflow cycle is imperative for efficient energy recovery. Nanoporosity and addition of concentrated electrolytes are critical for improved storage density and lower kinetic barriers to the liquid expulsion. Our molecular simulations provide a theoretical perspective into the mechanisms involved in the process, and underlying structures and interactions in compressed nanoconfined solutions. Specifically, we consider aqueous NaCl in planar confinements of widths of 1-2 nm and pressures of up to 3 kbar. Open ensemble Monte Carlo simulations with fractional exchanges of ions are utilized in conjunction with pressure-dependent chemical potentials of bulk phases under pressure. Confinements open to pressurized bulk electrolyte phases show improved reversibility enabled by significant increases in the solid/liquid interfacial tension in narrower pores and associated infiltration and expulsion pressures. These changes are consistent with a strong desalination effects observed in the nanopores irrespective of external pressure and initial concentration.

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