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Structure and Capacitance of Electrical Double Layers inside Micropores GUANG FENG, RUI QIAO, JINGSONG HUANG, BOBBY G. SUMPTER, VINCENT MEUNIER, ME@CU TEAM, ORNL COLLABORATION — Recent experiments indicate that the specific capacitance of micropores (diameter less than 2nm) increases anomalously as the pore size decreases^[1]. To understand the physical origin of this discovery, we performed a series of molecular dynamics simulations to study the electrical double layers (EDLs) in micropores with different shapes (tube vs slit) and pore sizes (0.668nm - 3.342nm). Several different aqueous electrolytes (K^+ , Na^+ , Cl^- , and F^- in water) were used in these micropores. We quantified the structure of EDLs inside the pores, and computed the capacitance of EDLs. The scaling of capacitance shows a qualitative agreement with the experimental observations. We attribute the anomalous enhancement of capacitance in micropores to the short-range ion-electrode and ion-solvent interactions.[1] J. Chmiola, G. Yushin, Y. Gogotsi, C. Portet, P. Simon, and P.L. Taberna, Science 2006, 313, 1760.

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