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Charging Dynamics of Sub-nanometer Pores YING LIU, Clemson University, GUANG FENG, JINGSONG HUANG, BOBBY SUMPTER, Oak Ridge National Laboratory, VINCENT MEUNIER, Rensselaer Polytechnic Institute, RUI QIAO, Clemson University — Electrodes featuring sub-nanometer pores can potentially improve the energy density of supercapacitors significantly. However, ions entering such narrow pores often need to pay an energy penalty because part of their salvation shell must be removed. This can potentially limit the charging kinetics of such nanopores. In this work, we investigate the charging dynamics of sub-nanometer pores connected with an electrolyte bath. We quantify the energy barrier for ions to enter 0.82-nm wide slit pores and determine the time constant for charging of the pores using Molecular Dynamics simulations. Strong concentration polarization is found during the charging process and the charging kinetics is much slower than that predicted using the classical equivalent circuit model. The results are rationalized using a modified Poisson-Nernst-Planck model.

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