

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Molecular Simulations of Graphene-Based Electric Double-Layer Capacitors**<sup>1</sup> RAJA K. KALLURI, DEEPTHI KONATHAM, ALBERTO STRIOLO, The University of Oklahoma, School of Chemical, Biological and Materials Engineering — Towards deploying renewable energy sources it is crucial to develop efficient and cost-effective technologies to store electricity. Traditional batteries are plagued by a number of practical problems that at present limit their widespread applicability. One possible solution is represented by electric double-layer capacitors (EDLCs). To deploy EDLCs at the large scale it is necessary to better understand how electrolytes pack and diffuse within narrow charged pores. We present here simulation results for the concentrated aqueous solutions of NaCl, CsCl, and NaI confined within charged graphene-based porous materials. We discuss how the structure of confined water, the salt concentration, the ions size, and the surface charge density determine the accumulation of electrolytes within the porous network. Our results, compared to data available for bulk systems, are critical for relating macroscopic observations to molecular-level properties of the confined working fluids.

<sup>1</sup>Research supported by the Department of Energy.

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Date submitted: 22 Nov 2010

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