

# Molecular Insights into Electrical Double Layers in Graphene-Based Supercapacitors

Sheng Bi,<sup>1</sup> Guang Feng,<sup>1,\*</sup> Song Li,<sup>1</sup> Nina Balke,<sup>2</sup> Peter T. Cummings,<sup>3</sup> Rui Qiao,<sup>4</sup> Alexei A. Kornyshev<sup>5</sup>

<sup>1</sup>State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan, Hubei 430074 China

<sup>2</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

<sup>3</sup>Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN 37235, USA

<sup>4</sup>Department of Mechanical Engineering, Virginia Tech, Blacksburg, Virginia 24061, USA

<sup>5</sup>Department of Chemistry, Imperial College London, SW7 2AZ London, UK

Corresponding Author. Email: [gfeng@hust.edu.cn](mailto:gfeng@hust.edu.cn)

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## Abstract

Recently nano-structural carbons have become the most widely used electrode materials in supercapacitor community, because of their high specific surface area, good electrical conductivity, chemical stability in a variety of electrolytes, and relatively low cost. In particular, graphene-based carbons are emerging as an auspicious candidate due to the unique feature of graphene. Among electrolytes used for supercapacitors, ionic liquids (ILs) have been becoming a promising class of them, owing to their exceptionally wide electrochemical stability window, excellent thermal stability, non-volatility and relatively inert nature. Despite considerable work on supercapacitor with graphene-based carbon as electrodes, the details of what happens under nano-confinement, including pores, still require in-depth exploration especially for IL electrolytes.

We studied the interfacial phenomena occurring between ILs and graphene-based electrodes in supercapacitors, using the combined molecular dynamics (MD) simulation by modeling ILs-based EDLs at planar, cylindrical, spherical electrode surfaces and inside electrode pores at nano/micro-scale. This talk would include:

1) MD modeling on ILs-based EDLs at open surfaces (e.g., planar, cylindrical, spherical, with defects, etc.) [1-2] and the integration with experiments (e.g., atomic force microscopy, AFM) [3-4], which would focus on the EDL structure and its influence from ion size, ion type, applied potential, electrode curvature, etc.

2) MD modeling on ILs-based porous carbon supercapacitors [5-7], which would embody the pore size effects on capacitance, the ion dynamics under porous confinement, and pore expansion during charging.

3) The anatomy of electrosorption for water in ionic liquids at electrified interfaces [8], which would show, for the first time, the work on the adsorption of water on electrode surfaces in contact with humid ILs.

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