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Atomic Probing Structures of Electrolytes at Graphene Surface: Insights from X-ray Scattering and Molecular Dynamics

HUA ZHOU, PAUL FENTER, Argonne National Laboratory, PANCHAPAKESAN GANESH, PAUL KENT, DEEN JIANG, ARIEL CHIALVO, PASQUALE FULVIO, SHENG DAI, Oak Ridge National Laboratory, GUANG FENG, MICHAEL ROUHA, PETER CUMMINGS, Vanderbilt University, VOLKER PRESSER, JAKE MCDONOUGH, YURI GOGOTSI, MATTHEW WANDER, KEVIN SHUFORD, Drexel University — The interactions of electrolyte fluids with carbon-based electrodes control many complex interfacial processes encountered in electrochemical energy storage systems. However, our knowledge of the atomic/nanoscale reactivity at interfaces of electrolytes with electrodes remain scarce due to the incomplete understanding of interfacial structures and processes in-situ and real-time encountered in real operation conditions. In this talk, we will present our efforts to obtain a molecular-scale perspective of the interactions of electrolytes with carbon surfaces near “real world” conditions. Structures of various electrolytes including salt aqueous and ionic liquids on atomically flat graphene (epitaxially grown on a SiC substrate), an ideal model fluid-solid interface system, were investigated by coupling high-resolution interface X-ray scattering techniques with molecular modeling-simulation approaches. These results provide a base-line for understanding relevant electrolyte/carbon interactions and will lead to fundamentally new insights and provide unique tests of atomistic fluid-solid interface models for energy storage systems.

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