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How Water Meets Graphene HUA ZHOU, PAUL FENTER, Argonne National Laboratory, JAKE MCDONOUGH, VOLKER PRESSER, YURI GOGOTSI, Department of Materials Science and Engineering, Drexel University, MATTHEW WANDER, KEVIN SHUFORD, Department of Chemistry, Drexel University — The interactions of electrolyte fluids with solids control many complex interfacial processes encountered in electrochemical energy storage systems. In this talk, we will demonstrate how to develop a fundamental atomic-scale understanding of interfacial structures at the water-graphene interface, a model fluid-solid interface combination. We have performed systematic measurements of high resolution X-ray reflectivity from epitaxial graphene films in contact with electrolytes including deionized water and aqueous salt solutions. The electron density profiles and structural models from the fully analyzed data reveal the intrinsic interfacial structures. It is noted that the interfacial water structure above the first graphene layer exhibits remarkable differences with those of subsequent graphene layers. The latter one, resembling water on freestanding graphene, is well predicted by parallel computational simulations. Moreover, the pH of aqueous solutions was found to have a subtle influence on the interfacial water structure above the first graphene layer. This may well be an indication of the interfacial structural distortions that might exist in this layer, and which may play an important role in controlling the chemical activity of monolayer epitaxial graphene.

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