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Simulation study on structure of water in aqueous solutions confined between graphene electrodes under very high applied electric field¹ GARY LEUTY, MESFIN TSIGE, The University of Akron, SAIKAT TALAPA-TRA, Southern Illinois University at Carbondale — Arising from questions regarding electric double-layer capacitors utilizing graphene electrodes and aqueous electrolyte (KOH solution), atomistic MD simulations of electrolyte confined between graphene electrodes were performed to understand the behavior of electrolyte as a function of electric field strength and solution concentration, from pure water to 6M KOH. It was noted that the strength of the electric field had a demonstrable effect on the structure of pure water between the electrodes (as has previously been seen in highly confined multilayer water systems), creating regularly spaced channels and densely packed sheets of highly ordered molecules. We also saw a clear effect due to the presence of electrolyte ions and their separation from the water due to the action of the field; different field strengths appear to greatly alter the distribution of ions, which in turn affects the structure and ordering of the water. Time dependence in the strength of the electric field was also studied to determine what effect, if any, it has on induced structure.

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