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The Effect of Polarization on Structure, Dynamics and Electric Double Layer for Interfacial Water near Charged Graphene[1] ALBERTO STRIOLO, TUAN A. HO, The University of Oklahoma, MOLECULAR SCIENCE AND ENGINEERING TEAM TEAM — A solid surface perturbs water for up to 10-20 Å. Quantifying the structural and dynamics properties of water within this interfacial layer remains crucial for a number of applications, including lab-on-chip and micro- and nano-fluidic devices, and also for designing efficient electric double layers capacitor. As graphene is finding wide applications in the energy sector (batteries and capacitors) we revisited the graphene-water interface. Because at the air-water interface it is known that accounting for the polarization of water and ions is required to properly describe the ions distribution, we conducted a parametric study in which we varied the polarization of carbon atoms on charged graphene. The polarization is described implementing a classic Drude oscillator, which is consistent with the model implemented to describe water and ions. External electric fields are represented by uniform charge distributions on the carbon atoms. The results are quantified in terms of structure and dynamics of interfacial water, as well as of structure of the electric double layer. Comparison with accurate experimental observations is provided.

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