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Molecular structure and polarization of water interfaces: physical picture from the hydrogen bonding of constrained geometry SUCHEOL SHIN, ADAM WILLARD, Massachusetts Institute of Technology — In this talk, we highlight the fundamental relationship between hydrogen bonding and aqueous interfacial molecular polarization. We describe this relationship, and how it is mediated by the density profile of water interface, in terms of a mean field model of interfacial hydrogen bonding. Specifically the model can predict the orientational distribution of interfacial water molecules based on the anisotropic local density and given hydrogen bond geometry. We demonstrate that the fluctuation in bond geometry at the interface is fairly different from that in the bulk environment and it is closely related with the mean polarization and its mean fluctuation observed at the interface.

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