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标题: Profile of the Static Permittivity Tensor of Water at Interfaces: Consequences for Capacitance, Hydration Interaction and Ion Adsorption

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摘要: We derive the theoretical framework to calculate the dielectric response tensor and determine its components for water adjacent to hydrophilic and hydrophobic surfaces using molecular dynamics simulations. For the nonpolarizable water model used, linear response theory is found to be applicable up to an external perpendicular field strength of similar to 2 V/nm, which is well beyond the experimental dielectric breakdown threshold. The dipole contribution dominates the dielectric response parallel to the interface, whereas for the perpendicular component it is essential to keep the quadrupole and octupole terms. Including the space-dependent dielectric function in a mean-field description of the ion distribution at a single charged interface, we reproduce experimental values of the interfacial capacitance. At the same time, the dielectric function decreases the electrostatic part of the disjoining pressure between two charged surfaces, unlike previously thought. The difference in interfacial polarizability between hydrophilic and hydrophobic surfaces can be quantized in terms of the dielectric dividing surface. Using the dielectric dividing surface and the Gibbs dividing surface positions to estimate the free energy of a single ion close to an interface, ion-specific adsorption effects are found to be more pronounced at hydrophobic surfaces than at hydrophilic surfaces, in agreement with experimental trends.

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