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Dielectric Properties of Water at the Rutile (110) Surface.

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The dielectric properties of interfacial water adjacent to the rutile (110) surface were investigated by means of non-equilibrium molecular dynamics simulations. The dielectric behavior of water arises from its local density and molecular polarizability in response to an external field, and can be rationalized in terms of the number and strength of water-surface and water-water H-bonds. A particularly strong dielectric response was found in the first water layer which leads to overscreening of the external electric field and negative permittivity and this behavior cannot be accounted for by bulk-like relations used in implicit solvent models. However, the negative permittivity of the contact water layer is counterbalanced by the positive permittivities of the surface depletion layer and second structured water layers such that the calculated Stern layer capacitance for the rutile (110)-water interface is positive and compatible with experimental macroscopic titration data. Simulations were also conducted on the negatively charged rutile (110) surface in the presence of NaCl electrolyte and the corresponding electrostatic profiles were virtually identical to those from the pure water-neutral surface simulations. Importantly, this means that the electrostatic profile at the rutile (110) surface is dominated by the charge density of water rather than ionic species thus supporting the "water centric" view of aqueous electrical double layers.

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Modeling the Interface: Mineralogy, Environment and Energy Applications (08:30 AM - 12:00 PM)

Location: Dallas Convention Center

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