Molecular dynamics calculations on the complex dielectric constant of a water thin film embedded in quartz surfaces

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The molecular dynamics calculations using the revised KKY water model are employed to investigate the dielectric property of a water thin film of ca. 0.8 nm thickness embedded between low quartz. The static dielectric constant is one of the most important physical parameters, which rules the solubility of organic and inorganic substances. The calculation results show that total electric dipole moment of a water thin film is anisotropic and a nearly 30% decrease of the static dielectric constant is observed when water is embedded between quartz surfaces. This decrease of static dielectric constant might facilitate the precipitation of ions and the resulting in the decrease of electric conductivity of the fluids at grain boundaries. The dielectric dispersion domain of a water thin film shifted to low frequency domain compared with bulk water. This result denotes that water between quartz is structurized like ice.

Additionally, in order to investigate the thickness dependent dielectric constant, the calculation results of water thin films having different thickness will be reported.