

Effect of Surface Polarity on the Structure and Dynamics of Water in Nano-Scale Confinement

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Session 3, Talk 1 (1:00 PM)

We present a molecular dynamics simulation study of the structure and dynamics of water confined between silica surfaces using β -cristobalite as a model template. We scale the surface Coulombic charges by means of a dimensionless number, k , ranging from 0 to 1, and thereby can model systems ranging from hydrophobic apolar to hydrophilic, respectively. Both rotational and translational dynamics exhibit a non-monotonic dependence on k characterized by a maximum in the in-plane diffusion coefficient, D_{\parallel} , at values between 0.6 and 0.8, and a minimum in the rotational relaxation time, τ_R , at $k = 0.6$. The slow dynamics observed in proximity of the hydrophobic apolar ($k = 0.0$) surface are a consequence of β -cristobalite templating and ice-like water layer. The fully hydrophilic surfaces, on the other hand, result in slow interfacial dynamics due to the presence of dense but disordered water that forms strong hydrogen bonds with surface silanol groups. Confinement also induces decoupling between translational and rotational dynamics, as evidenced by the fact that τ_R attains values similar to that of the bulk, while D_{\parallel} is always lower than in the bulk. The decoupling is characterized by a more drastic reduction in the translational dynamics of water compared to rotational relaxation.