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Structure, Dynamics and Thermodynamics of Confined Water: a Computational Perspective

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The behavior of water in confining geometries with characteristic dimensions in the nm range is of interest in a wide range of scientific fields and technical applications, such as biological self-assembly and tribology. Recent computational work on water in nano-scale confinement by inorganic and biological surfaces sheds new light on the roles of surface chemistry and geometry on water structure, water phase behavior in hydrophobic confinement over broad ranges of temperature and pressure, the evolution from surface-influenced to bulk-like dynamics, the dependence of dynamics on surface polarity, the relationship between the mechanical properties of glassy water thin films and surface polarity, water structure in confinement by heterogeneous surfaces, and the control of surface hydrophobicity by coupling polarity and topography. Such studies help develop the physical understanding needed for the rational design of surfaces for practical applications.