National Institute of Technology Rourkela

Departmental Seminar

Seminar Title	: Conference Return Seminar on Effect of Superhydrophilic Cylindrical Confinement on Phase Transition of Water (Presented at Molecular Materials and Functions-2024, IIT Madras, Chennai)
Speaker	: Mr. Vikas Kumar Sinha (Phd, Roll No. 520ch1002)
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Venue	: New Seminar Hall
Date and Time	: 19 Dec 2024 (11.00 A.M.)
Abstract	: Recent studies using molecular dynamics (MD) simulations suggest that water under confinement has anomalous phase transition behavior compared to bulk water. Nanoscale-confined water has engendered intense interest because of its importance in materials science and biology. Here, we investigate the effect of superhydrophilic confinement on physical and thermodynamic properties (potential energy, density, entropy, enthalpy, specific heat capacity (Cp), radial distribution function (RDF), structural dynamics, and transition temperatures) associated with the water phase transition. Superhydrophilic surfaces (membranes) have applications in multiple-fields, including wastewater treatment, antifogging, antifouling, biotechnology, signaling activity, cellular functions, adhesion proteins, and proliferation. Strongly-hydrophilic confinement (extreme environments) might give new perspectives on cognizance of the biological processes. We performed MD simulations (cooling and heating within 100-350 K) for water confined under superhydrophilic cylindrical nanopore with radius R varying from 1.0 nm to 5.0 nm in order to determine the water properties during phase transition. The cylindrical confinement of water (mW model) is modeled using Lennard-Jones 9-3 interaction potential for the three water-wall interaction strength (wf), 4.184 kJ/mol, 5.23 kJ/mol, and 7.32 kJ/mol. The results indicate that the water properties are contingent on confinement and the strength of water-wall interaction. Due to the cooling and heating curves of potential energy, a hysteresis loop has been observed around the phase transition temperature. Similar to potential energy, a hysteresis loop is also observed for enthalpy, density, and entropy within the same temperature range. An abrupt change in Cp signifies the transition temperature, melting temperature during heating and freezing temperature during quenching. Entropy increases with increasing the pore radius and decreases with increasing water-wall interaction, which agrees with previous literature. Structural analysis suggests that the variation in transition temperature might be due to differences in the crystalline % with changing the pore radius and the interaction strength of water-wall surfaces. Melting and freezing temperatures of cylindrical confinement are lower and higher with respect to bulk water, respectively. For lower pore radius ($R < 3.5$ nm), melting temperatures oscillate more for all water-wall interactions, which stabilizes beyond $R > 3.5$ nm. Similar behavior is observed with freezing temperatures.