# National Institute of Technology Rourkela

## Departmental Seminar

Seminar Title : Conference Return Seminar on Superhydrophilic Cylindrical Confinement Effect on Solid-Liquid Coexistence of Water Through Free Energy Analysis
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Venue : New Seminar Hall
Date and Time : 24 Mar 2025 (11.00 A.M.)

Abstract :

In contrast to bulk water, confined water exhibits distinct properties that make it more enthralling to explore, in particular the phase transition. Study of confined water systems is of colossal interest for several reasons, including the essence of understanding biological systems, further free energy calculation during phase transition is extremely important while studying chemical or biochemical phenomena including, macromolecular stability, protein folding, molecular solvation, and advancing drug discovery. However, earlier studies have typically emphasized hydrophobic or moderate hydrophilic confinement. Here, we explore the cylindrical confinement effect on solid-liquid coexistence of water within superhydrophilic pore with a radius (R) varying from 7.5 Å to 60 Å, through Gibbs free energy analysis using monatomic water (mW) model. We performed molecular dynamics simulations (LAMMPS) for determining the thermodynamic melting point or solid-liquid coexistence by employing multiple-histogram-reweighting (MHR) in conjunction with thermodynamic integration methods. By constructing a reversible and integrable path (pseudo-supercritical-transformation-path) which connects liquid and solid phases, the change in Gibbs free energy betwixt the phases is calculated for an approximate melting temperature (Tam). Each of the cylindrically-confined water systems has been simulated for the three wall-water interaction strengths ($\epsilon$): 1.17, 1.47, and 2.05 kcal/mol. Tam is evaluated from the hysteresis diagram of density-temperature curve. With increase in pore radius (or decrease in wall-water interaction strength), $\Delta G$ decreases (becomes more negative), signifies that melting process would be more spontaneous with increasing pore size (or decrease in wall-water interaction strength). Melting temperature is found to be increasing with increasing pore size and depressed with increase in wall-water interaction. However, for all the pore sizes with all three interaction strengths, the melting temperature is found to be lower compared to the recently reported melting point of bulk water. The study captivates reifying cavernous sagacity in the phase transition mechanism of water.