Thermodynamics of Liquids under Nanoconfinement

MUSE

Scientific Achievement

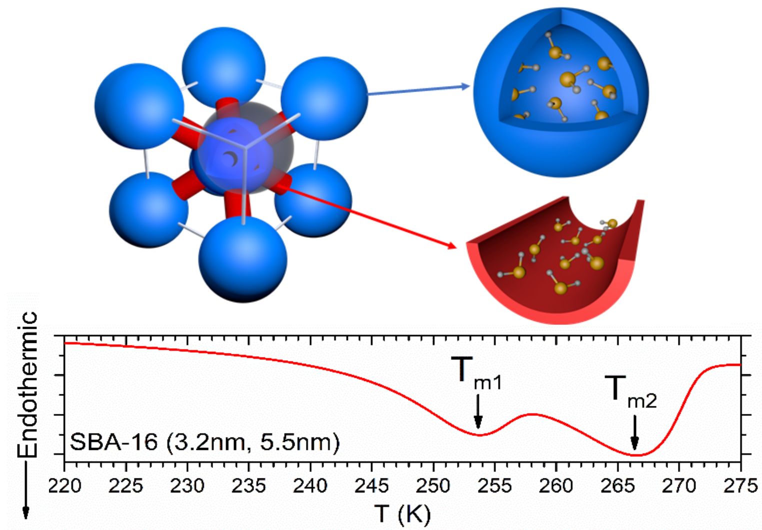
Extreme spatial heterogeneity and fluid-pore surface interactions are observed in the phase transition dynamics of liquids confined in nanoarchitected silica with interconnected pores of different geometry.

Significance and Impact

Results demonstrate that despite connectivity between the pores, nanoconfined fluids display distinct melting, boiling, and glass transition temperatures, characteristic of each pore type. Furthermore, simulations show that under weak fluid-pore interactions, the vapor pressure of confined hydrocarbons can exceed that of the bulk fluid.

Research Details

- Mesoporous silicas with bimodal pore geometries (SBA-16, FDU-5) were synthesized by acidic reaction methods.
- Melting, boiling, and glass transition temperatures were determined using differential scanning calorimetry (DSC).
- Gibbs Ensemble Monte Carlo (GEMC) simulations of confined liquids were performed for a range of pressures, surface chemistries, pore sizes and pore morphologies.



Top: Schematic pore structure of mesoporous silica SBA-16.
Bottom: DSC scans for D_2O confined in bimodal pores of SBA-16.

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-- Y. Xia, H. Cho, M. Deo, S. H. Risbud, M. H. Bartl, S. Sen, “Layer-by-Layer Freezing of Nanoconfined Water,” *Scientific Reports*, **2020**, 10, 5327.
-- Y. Xia, H. Cho, S. H. Risbud, M. H. Bartl, S. Sen, “Coexistence of Structural and Dynamical Heterogeneity in Liquids Under Nanoconfinement,” *Frontiers in Physics*, **2020**, 8, 130.
-- J. Li, Q. Rao, Y. Xia, M. Hoepfner, M. Deo, “Confinement-mediated Phase Behavior of Hydrocarbon Fluids: Insights from Monte Carlo Simulations,’’ *Langmuir*, **2020**, 36, 7277.

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