Motivation

Importance of porous materials:
- Catalysts
- Adsorbents
- Bio sensors
- Separation membranes

Research Objectives

- Understanding how the structure of the pore and molecular interactions determine fluid uptake
- Implement mean field theory (MFT) and dynamic mean field theory (DMFT) to model fluid adsorption in mesoporous materials.

Lattice Gas Model

- Lattice model of slit pores are useful for studying fluid adsorption in porous materials due to their simple geometry.
- Studying a variety of conditions shows different phenomena of fluid uptake in pores.

Thermodynamics

Adsorption/Desorption Isotherm: Length 32/33 width 6
- Hysteresis loops are predicted by the model due to meniscus formation.
- We pick what temperature to use for the dynamics based on the hysteresis position at that temperature.

Dynamics of Capillary Condensation

Dynamics: Length 32 width 6
- Single bridge formation evident from:
  - Sharp increase in the average density at the center
  - Difference in the two densities shown

Dynamics: Length 33 width 6
- Double bridge formation evident from:
  - Sharp decrease in the average density at the center
  - Density at the center drops below the average density across the pore and remains below it.

Summary

- Utilizing lattice model paired with MFT and DMFT to predict adsorption in a mesopore.
- Predicted bridging transition (single bridge to double bridge) as pore length is changed.
- Carried out a survey of thermodynamic and dynamic behavior for the slit pore for different lengths, widths and temperatures.

Future Work

- Modeling the adsorption/desorption of three dimensional ordered mesoporous carbon materials

References


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Dynamics: Length 32 width 6

Dynamics: Length 33 width 6

Adsorption/Desorption Isotherm: Length 32/33 width 6

DMFT - Evolution equation for the local density:

$$\frac{\partial \rho_i}{\partial t} = -\sum_{j} [w_{ij} \rho_j (1 - \rho_i) - w_{ji} \rho_i (1 - \rho_j)]$$