

Confinement Potential Inside Rare Gas Plated MCM-41 Nanopores

Nathan Nichols
(University of Vermont)

Timothy Prisk
(NIST)

Garfield Warren
(Indiana University Bloomington)

Paul Sokol
(Indiana University Bloomington)

Juan Vanegas
(University of Vermont)

Adrian Del Maestro
(University of Tennessee, Knoxville)

DMR-1809027

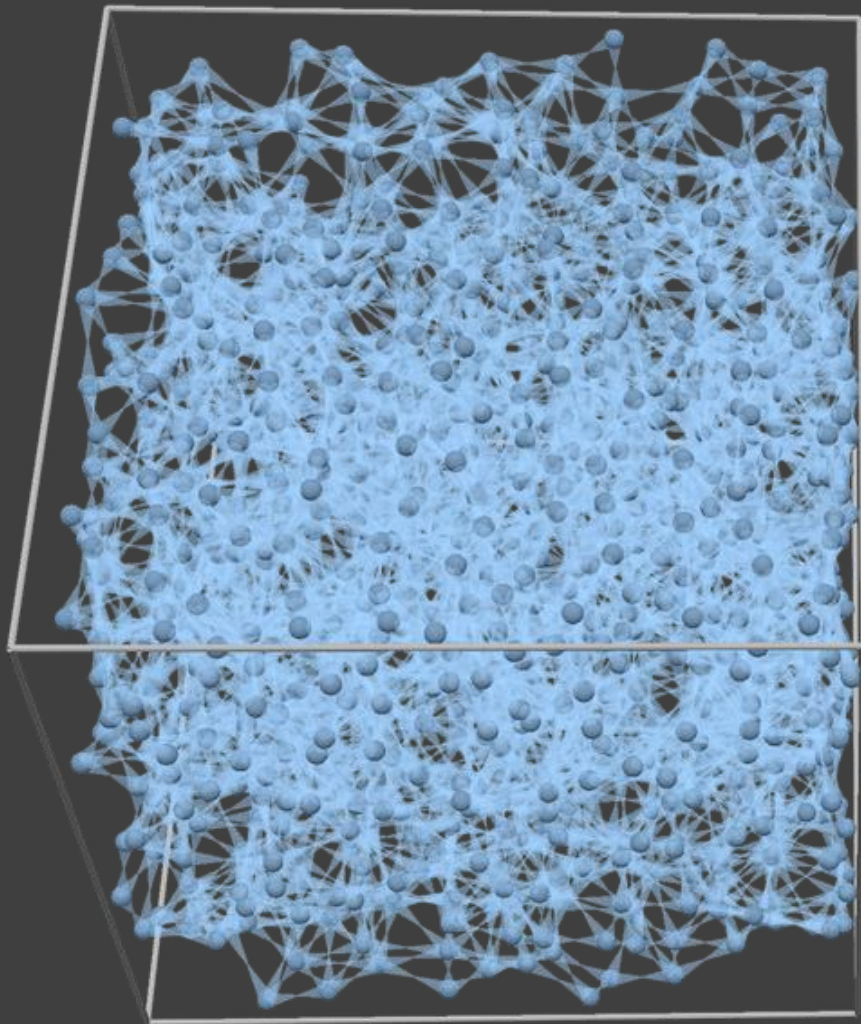
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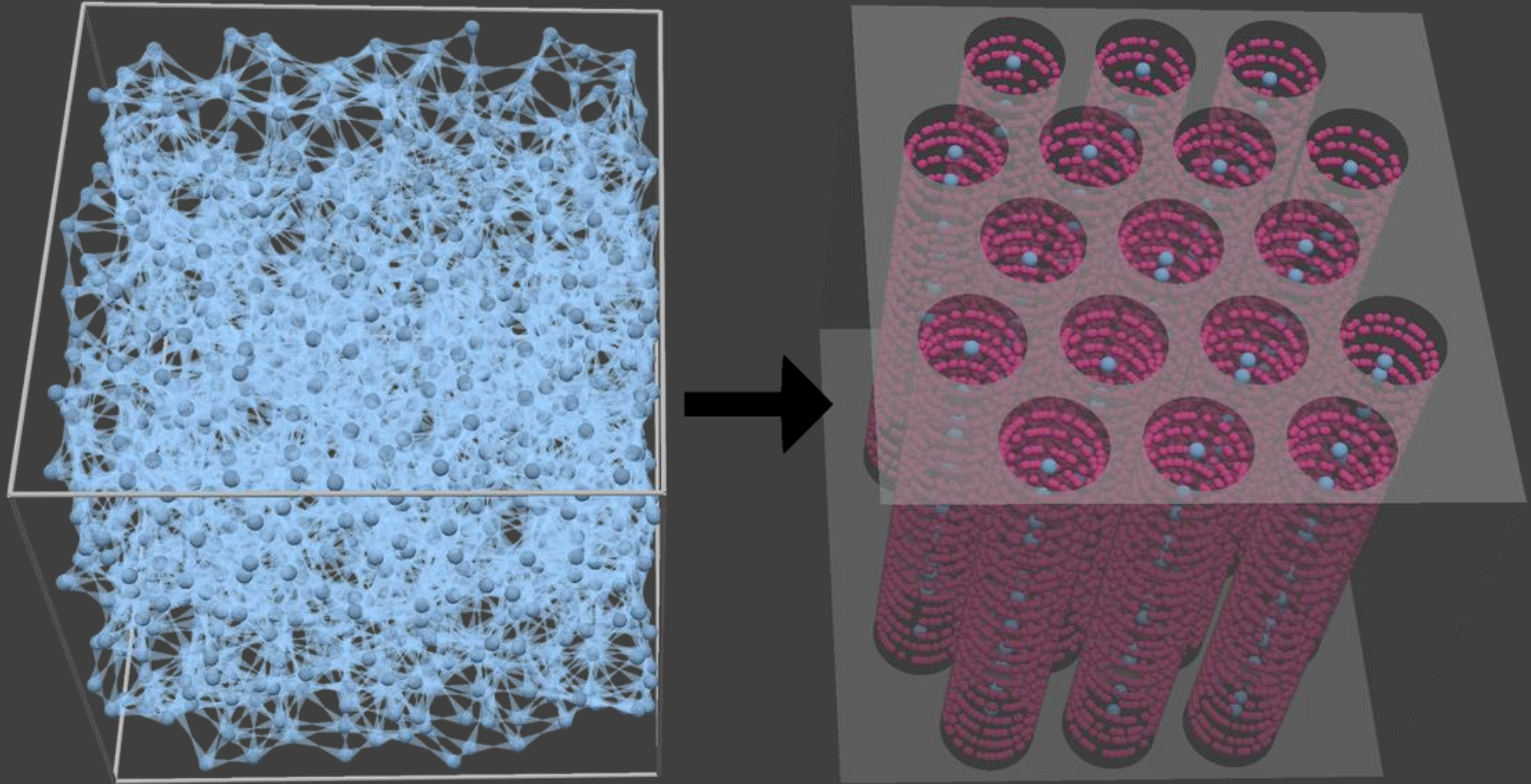


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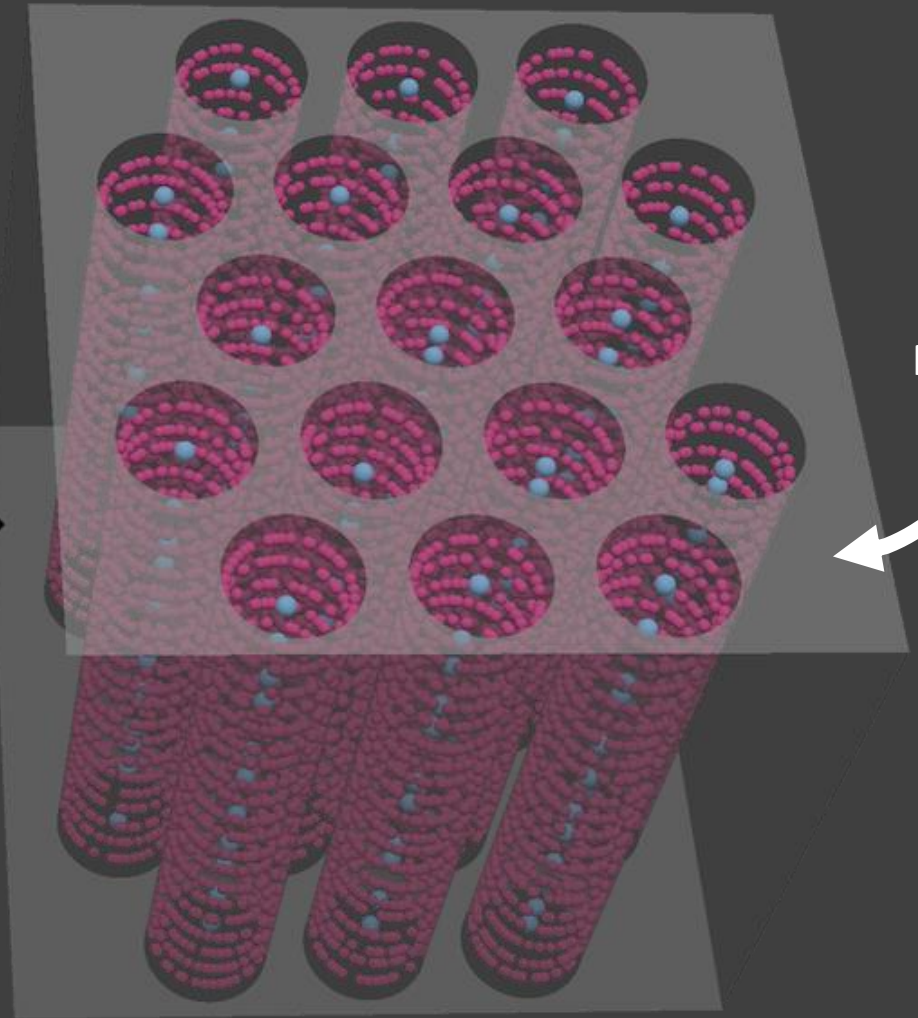
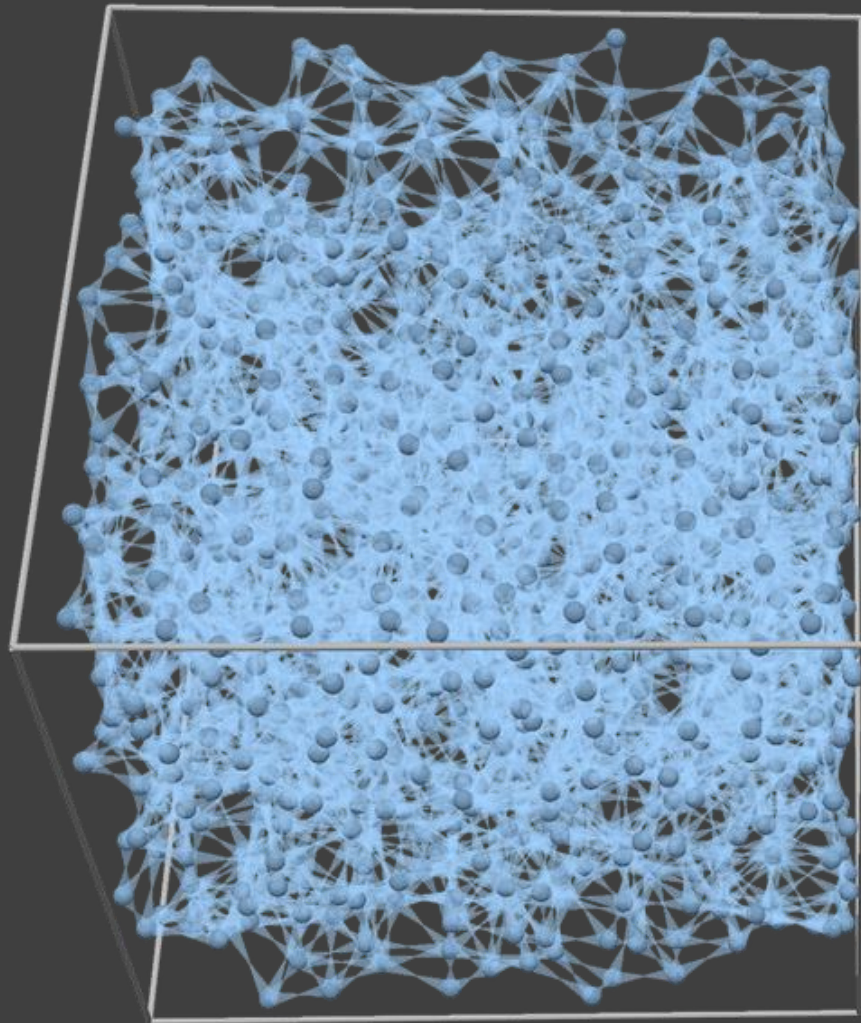
Dimensional Reduction of Bulk Helium-4



Dimensional Reduction of Bulk Helium-4



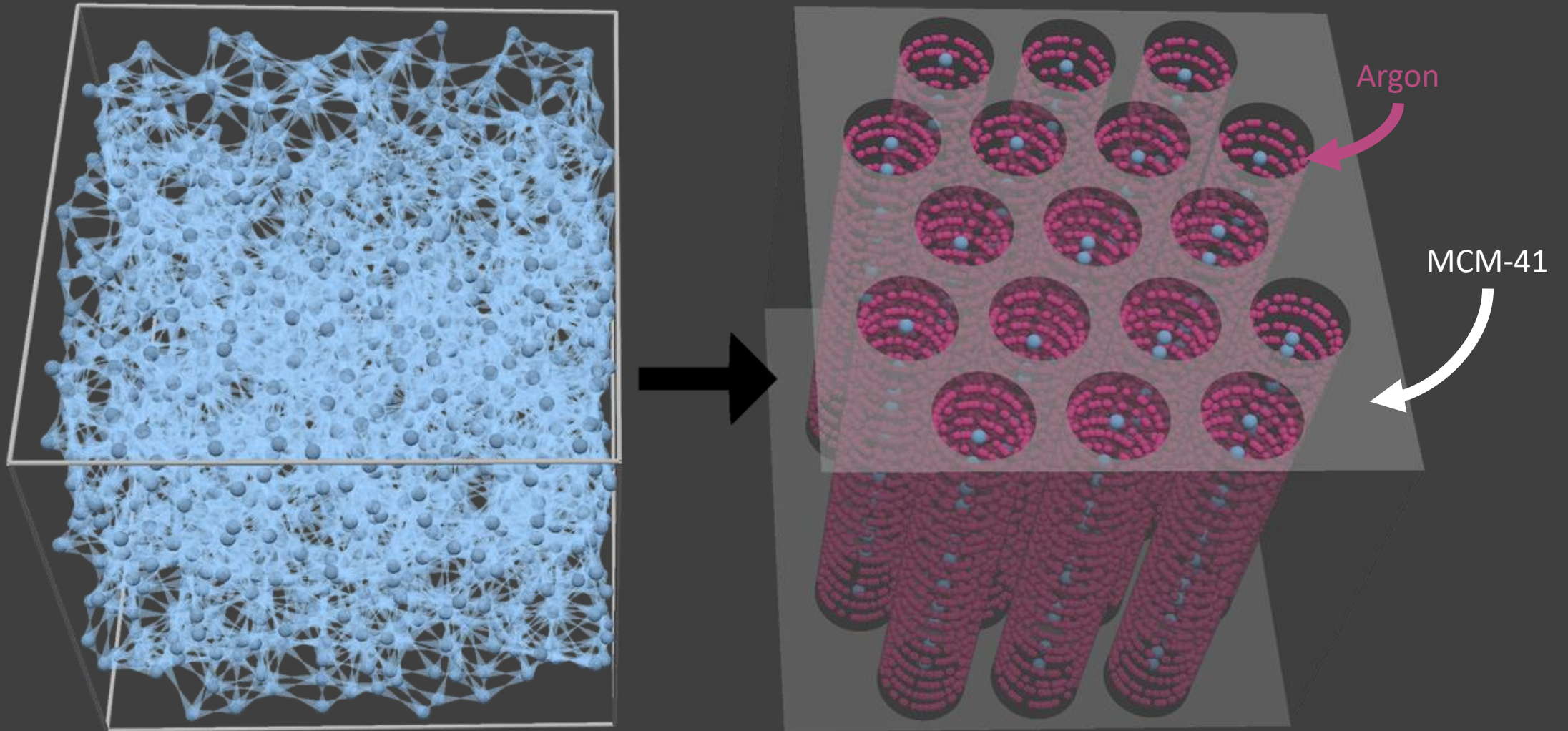
Dimensional Reduction of Bulk Helium-4



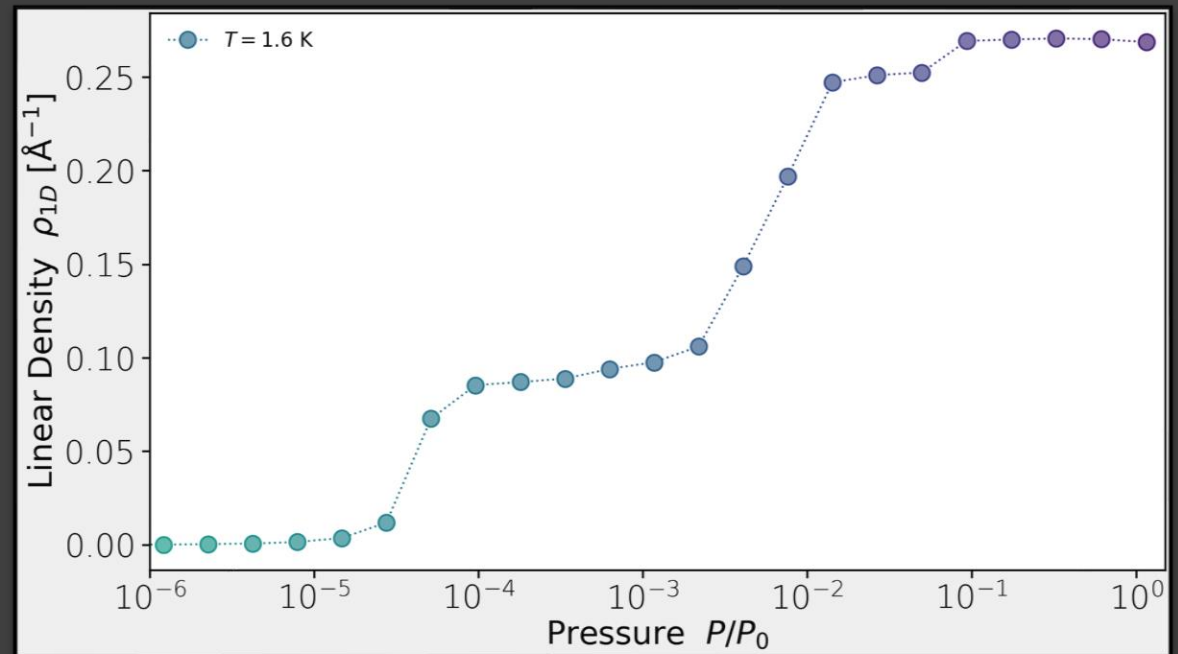
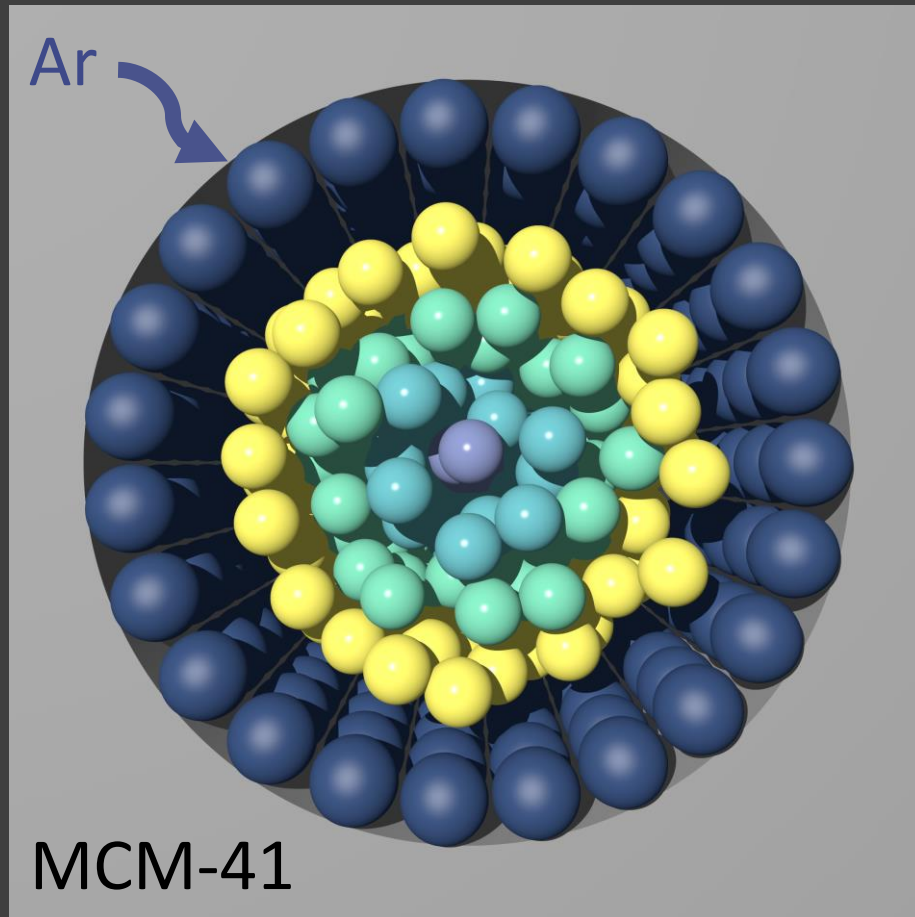
MCM-41



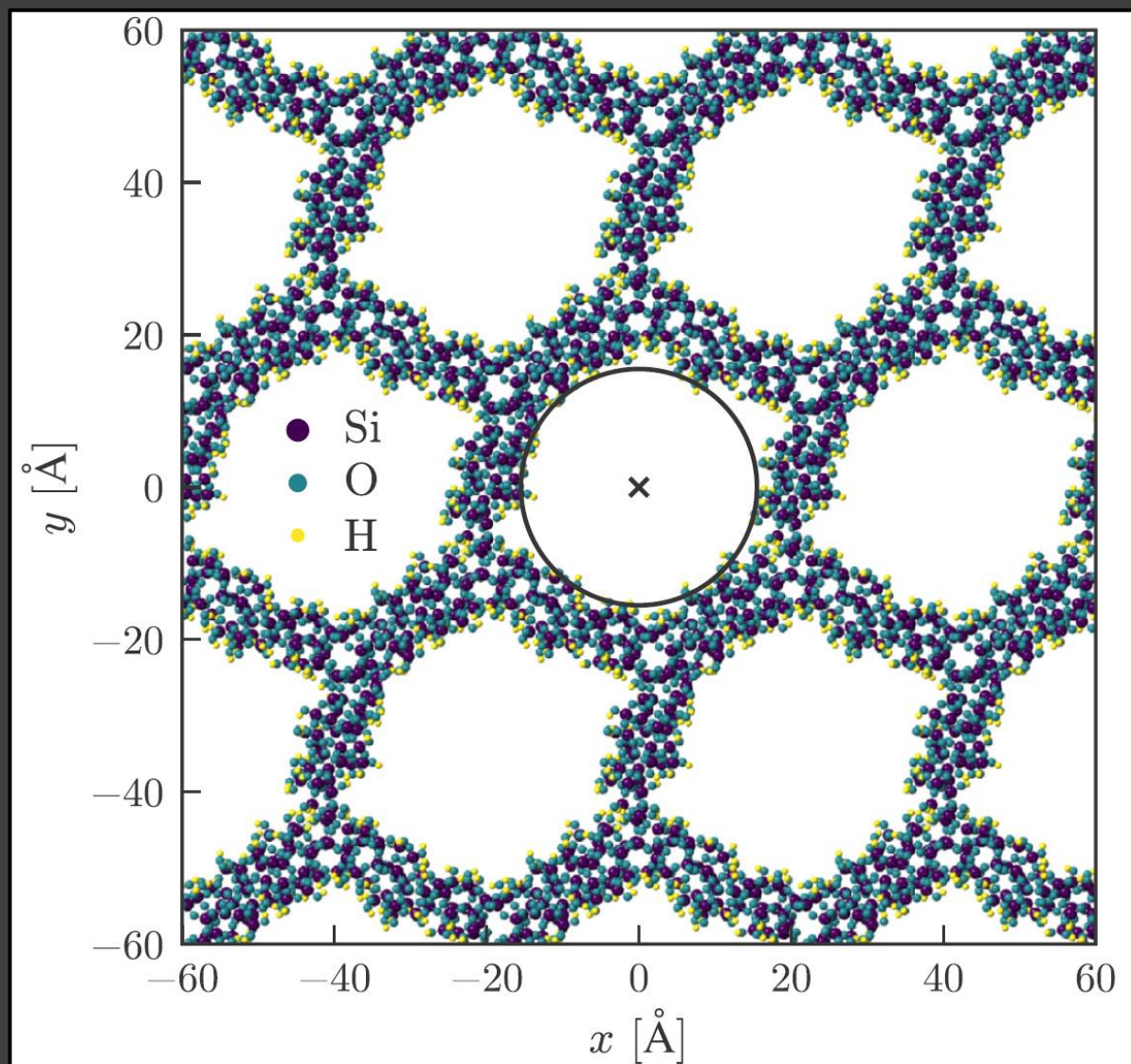
Dimensional Reduction of Bulk Helium-4



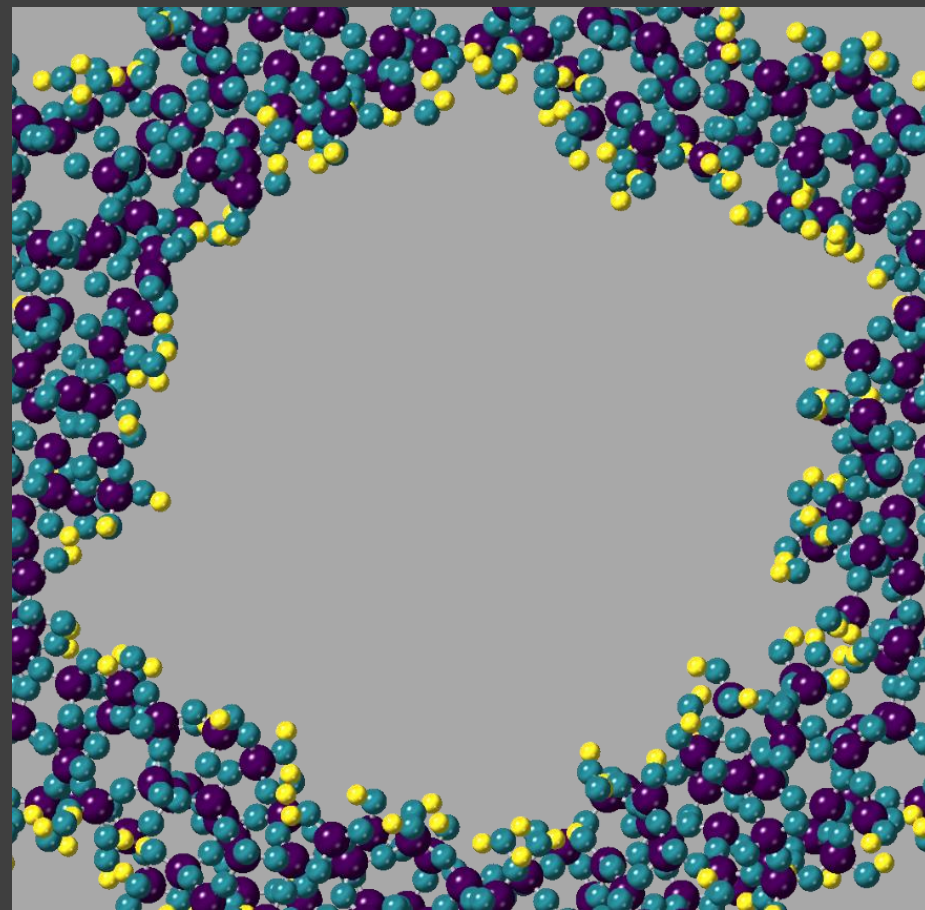
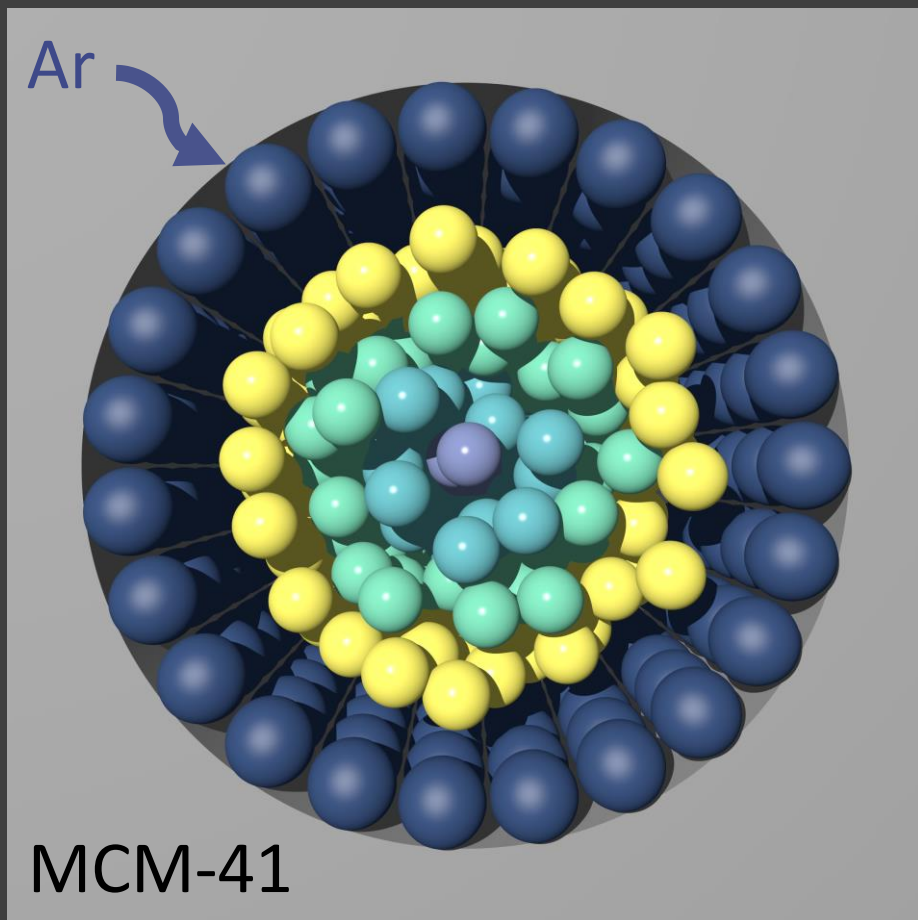
Linear Density of Central Core via QMC



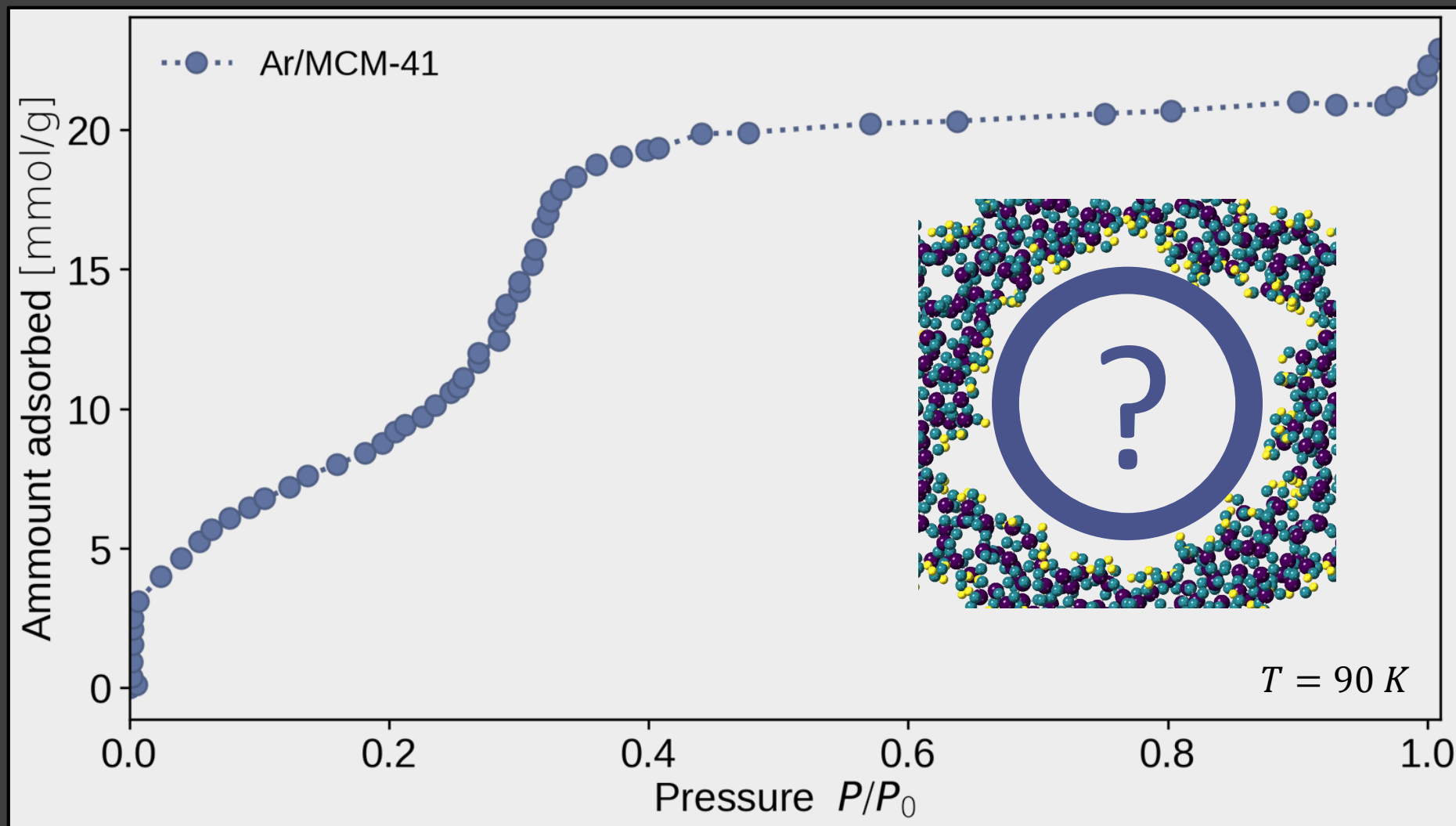
MCM-41 Crystal Structure



How smooth are those walls?

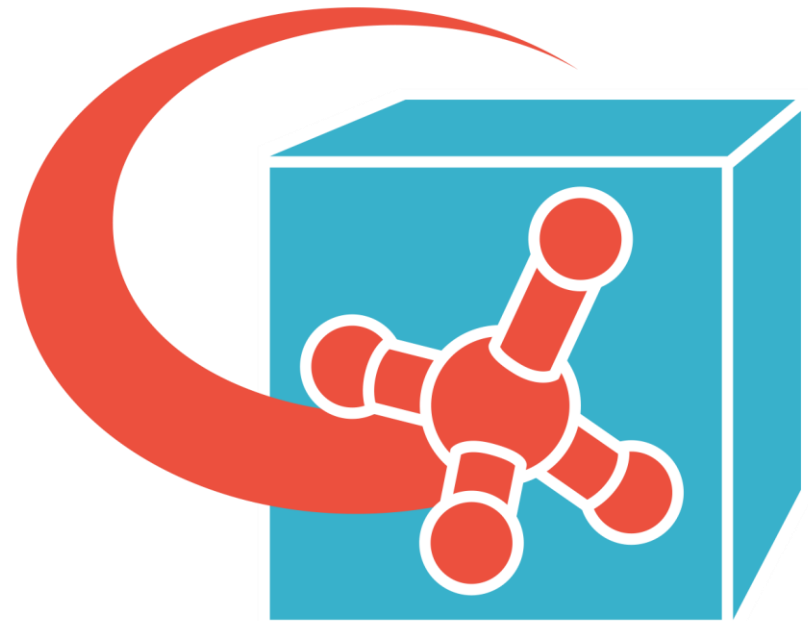


Experimental Argon Adsorption Isotherm



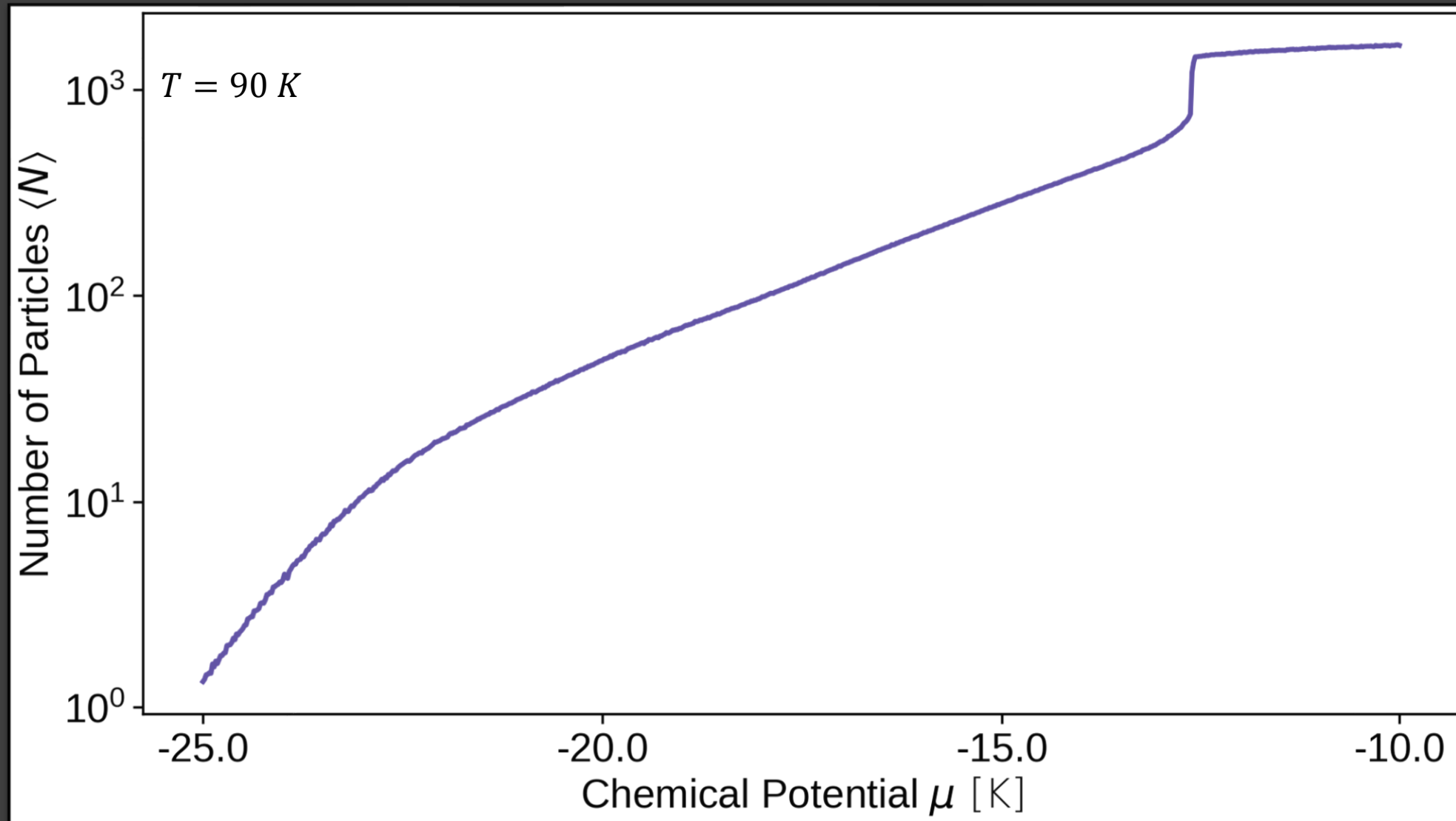
Cassandra

- Computational Atomistic Simulation Software At Notre Dame for Research Advances
- Many capabilities: NVT, NPT, **muVT**, NVT-Gibbs, NPT-Gibbs
- Grand canonical Monte Carlo simulations
 - Simulate argon in MCM-41 cell
 - Sweep over chemical potential
 - Generate adsorption isotherm

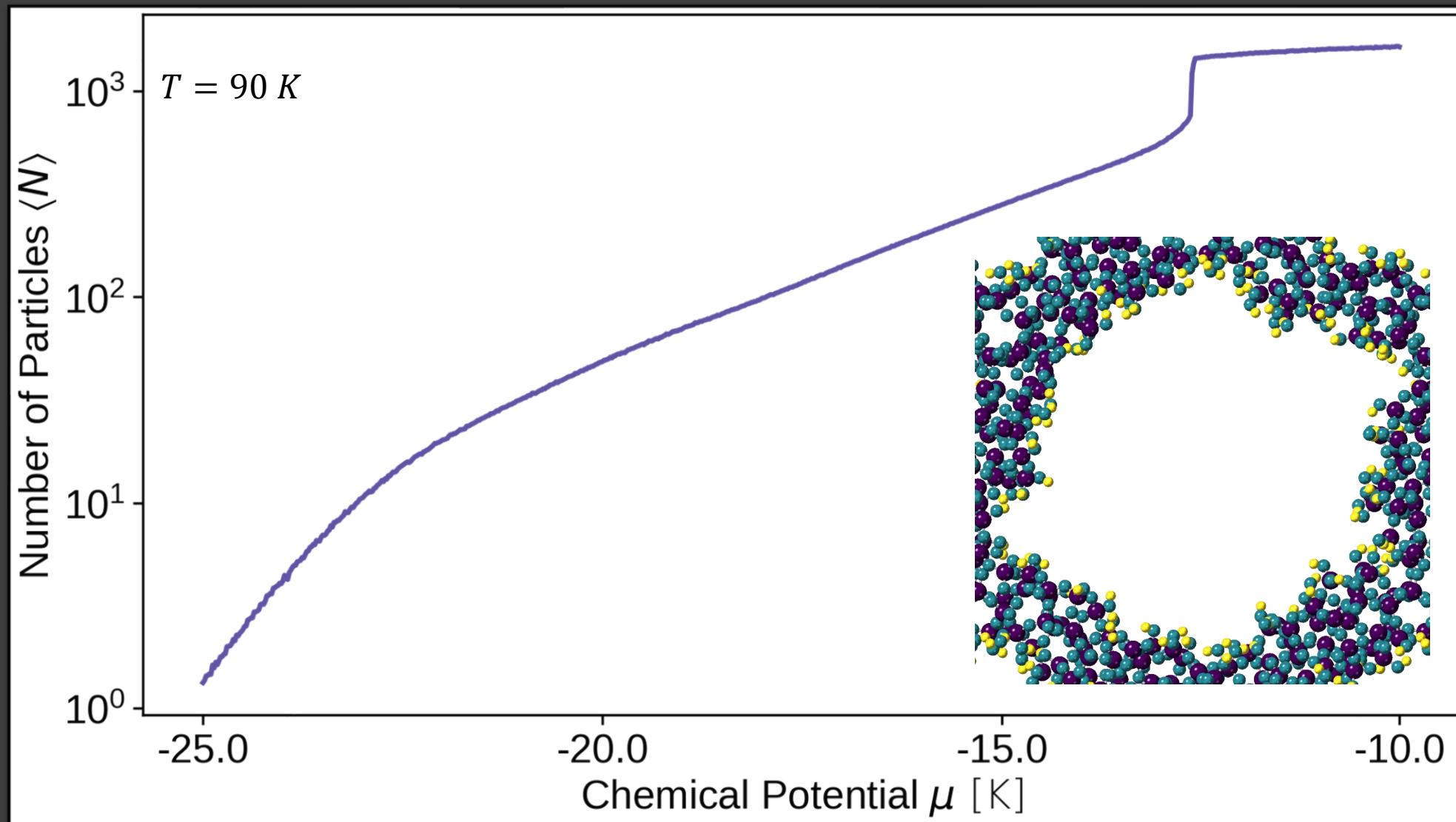


Cassandra
M o n t e C a r l o
S O F T W A R E

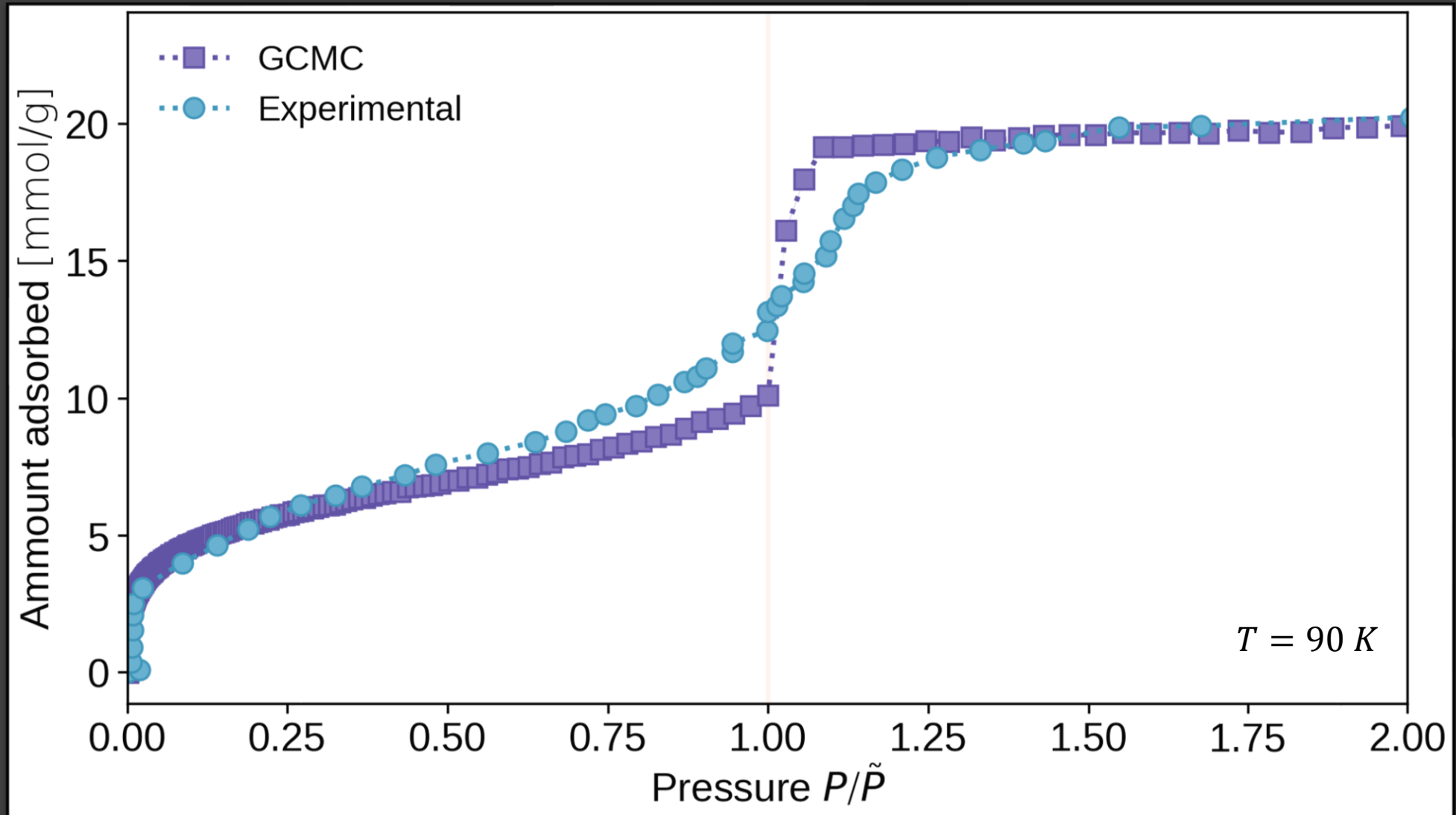
GCMC Argon Adsorption Isotherm



GCMC Argon Adsorption Isotherm



Adsorption Isotherm Comparison





Where is layer
completion?

Where is layer completion?

Use bulk modulus!

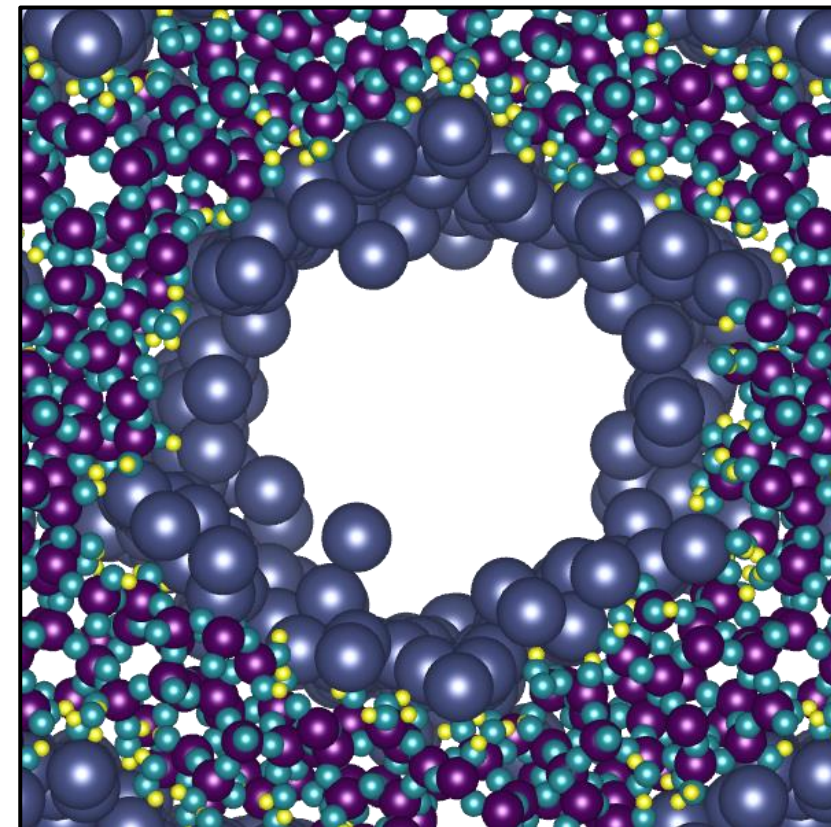
$$K = \rho k_B T \frac{\langle N \rangle}{\langle N \rangle^2 - \langle N^2 \rangle}$$

GROMACS

FAST.
FLEXIBLE.
FREE.



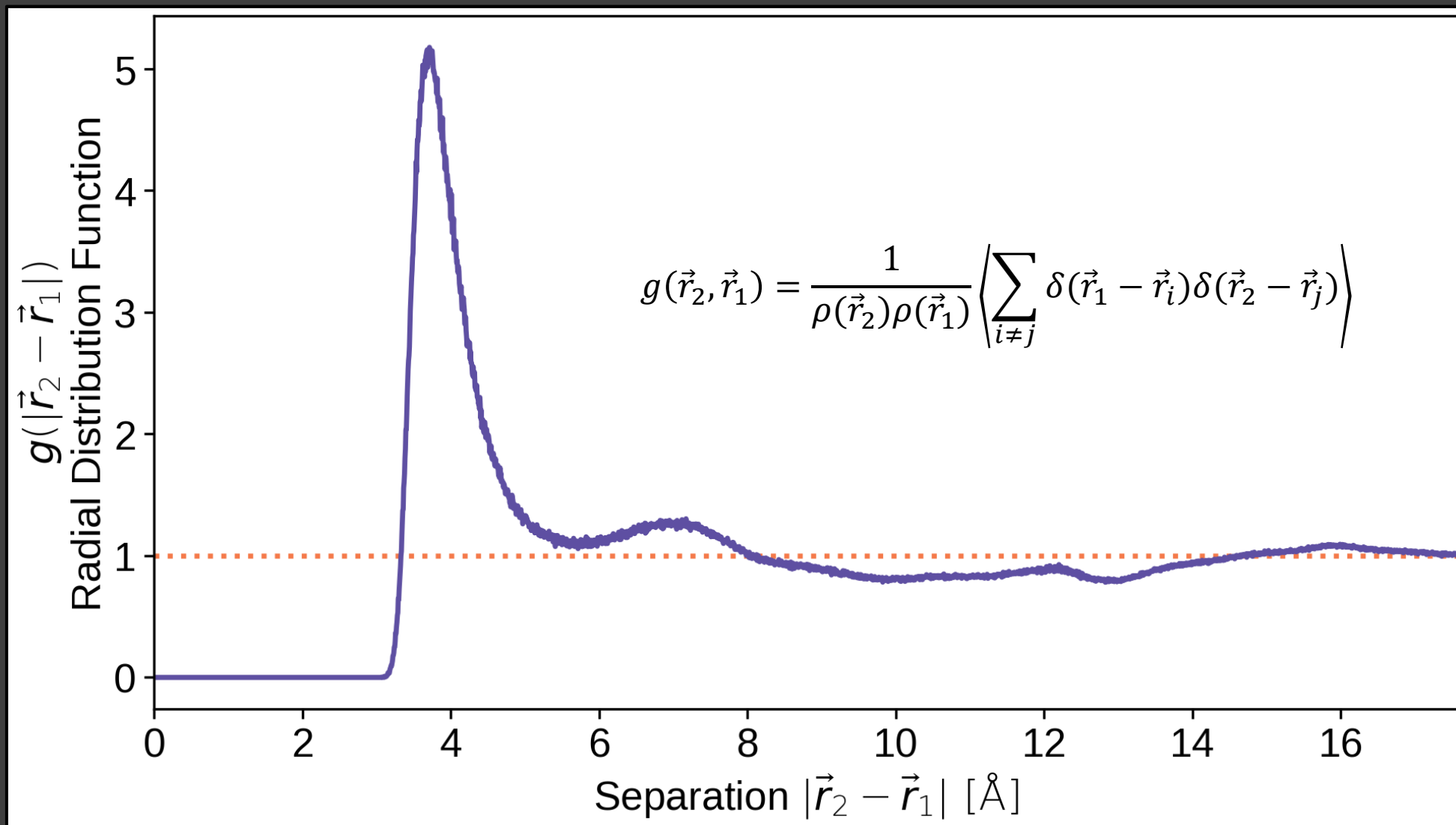
- Classical molecular dynamics simulations
- Parallel plus GPU support
- Test particle insertion
 - Use GCMC state file from Cassandra
 - Energy minimization of argon layer
 - Generate trajectory file
 - Insert helium and determine potential



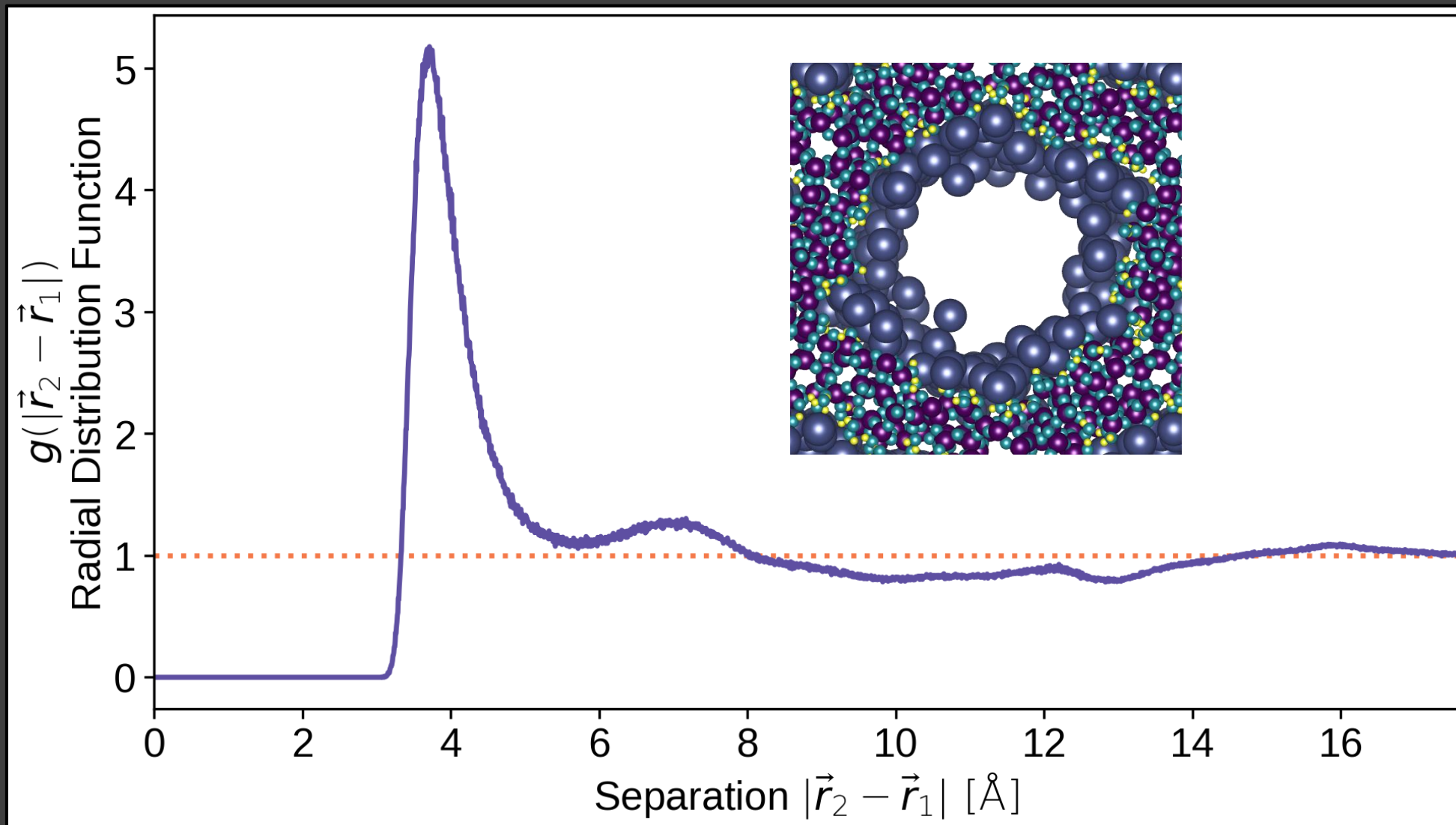
<https://www.gromacs.org/>

Szilárd et al. J. Chem. Phys., 153, 144505 (2020).

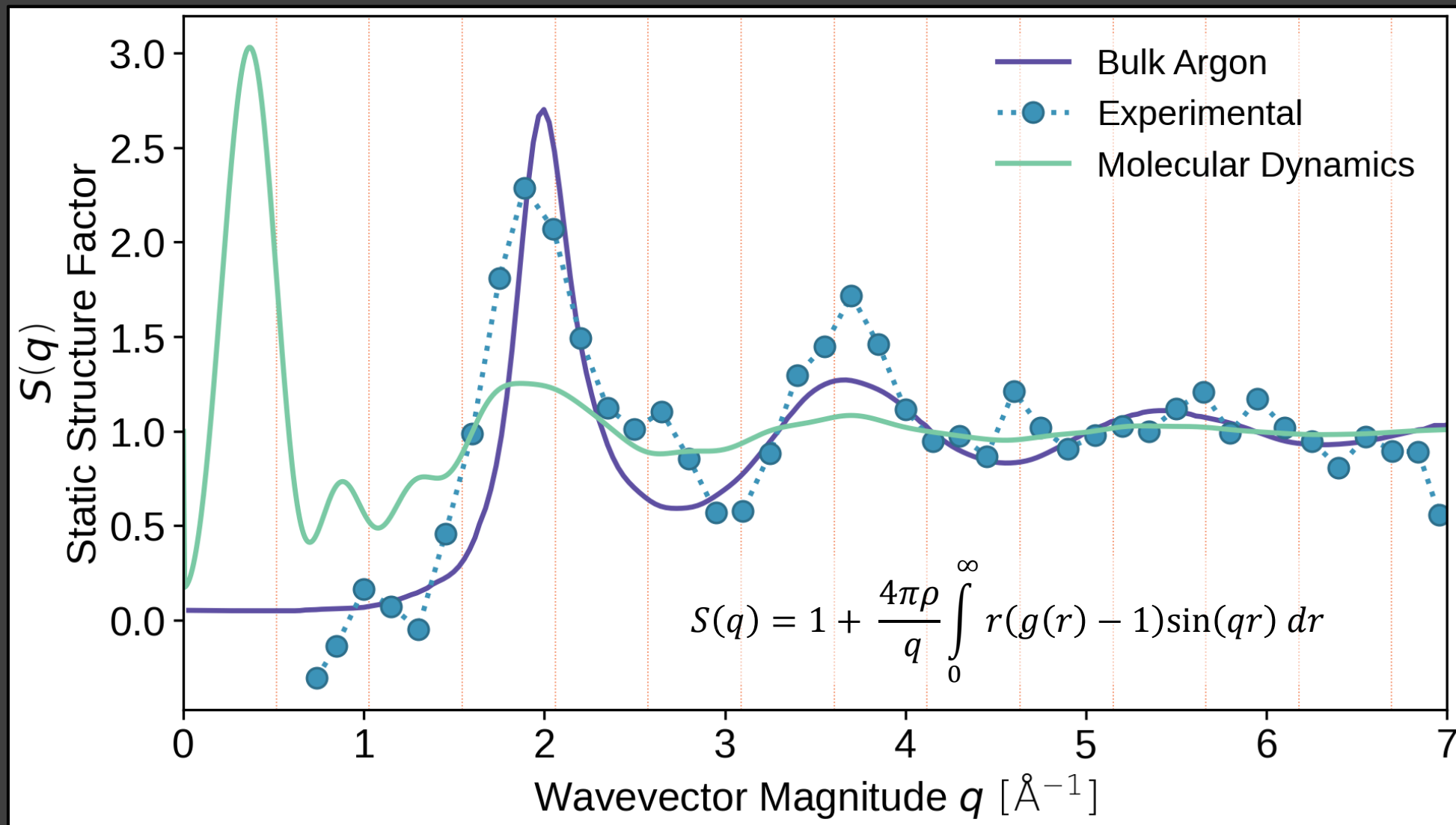
Radial Distribution Function



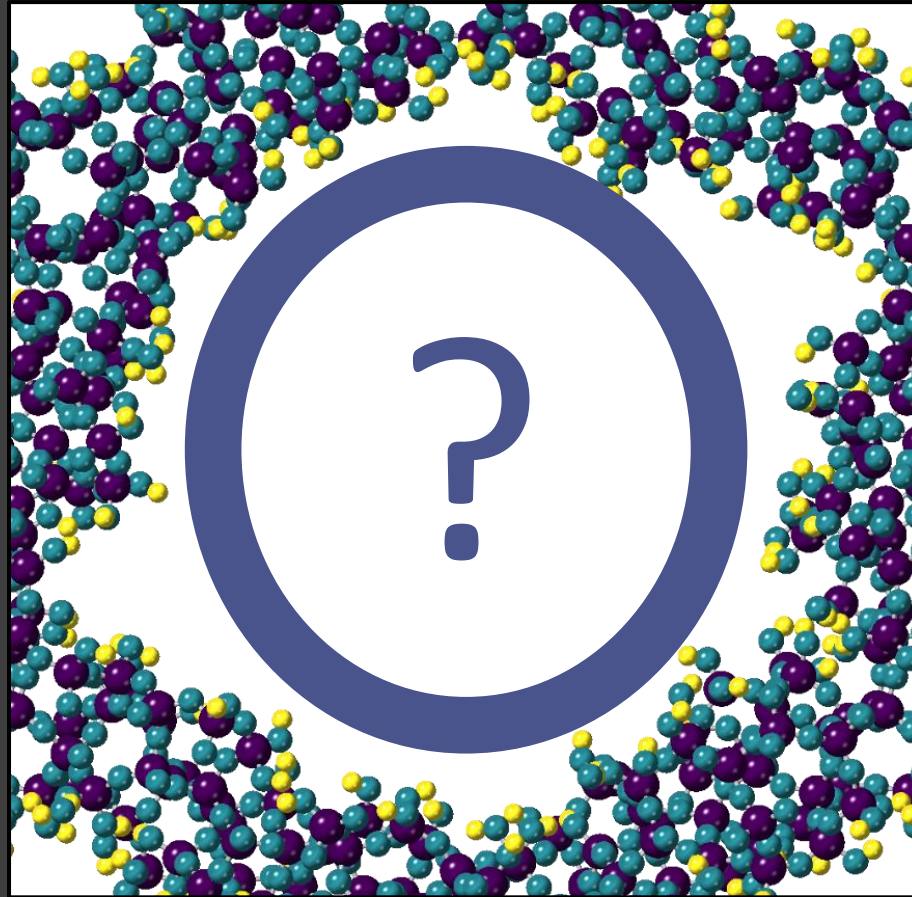
Radial Distribution Function



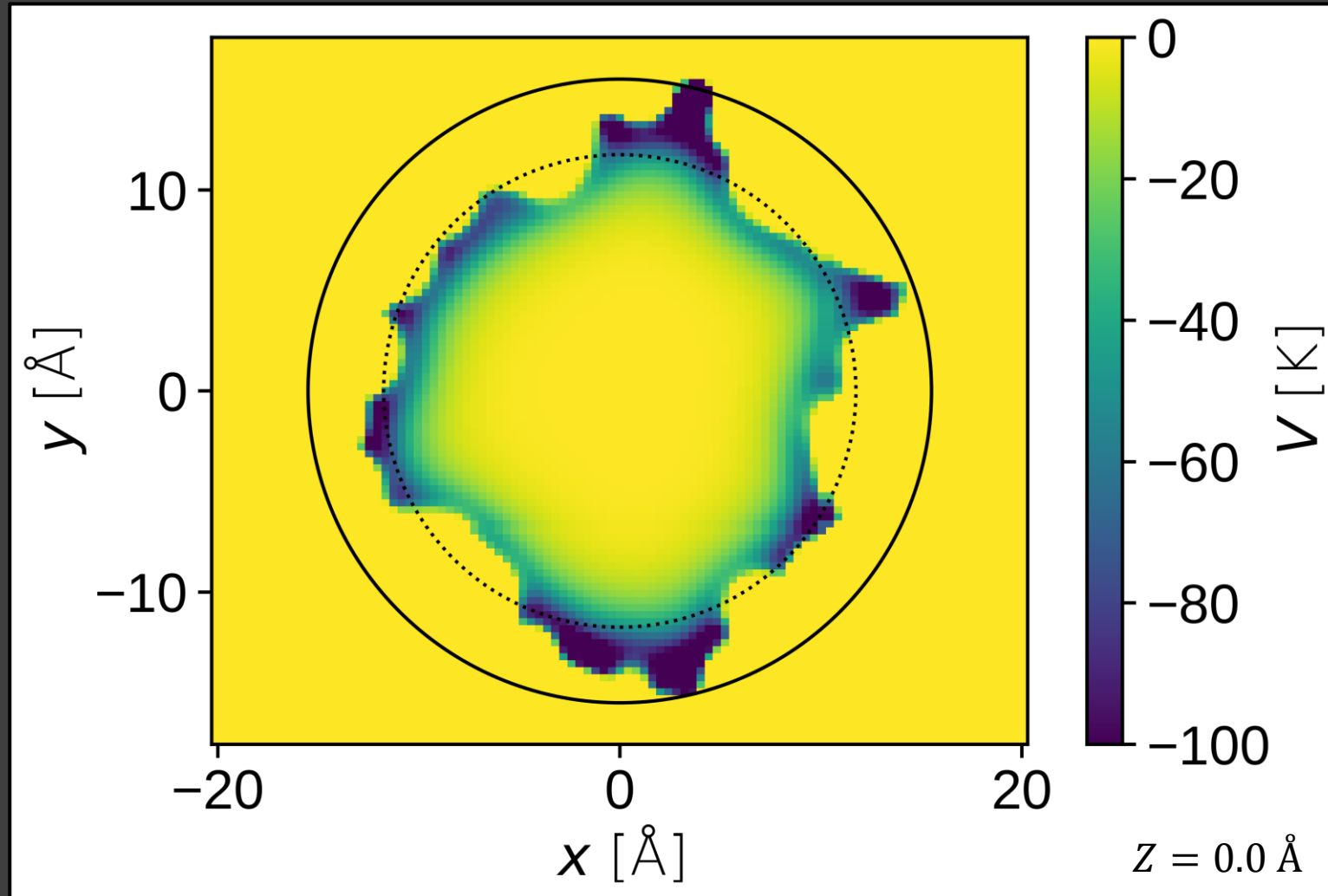
Static Structure Factor



Helium Test Particle Insertion Results

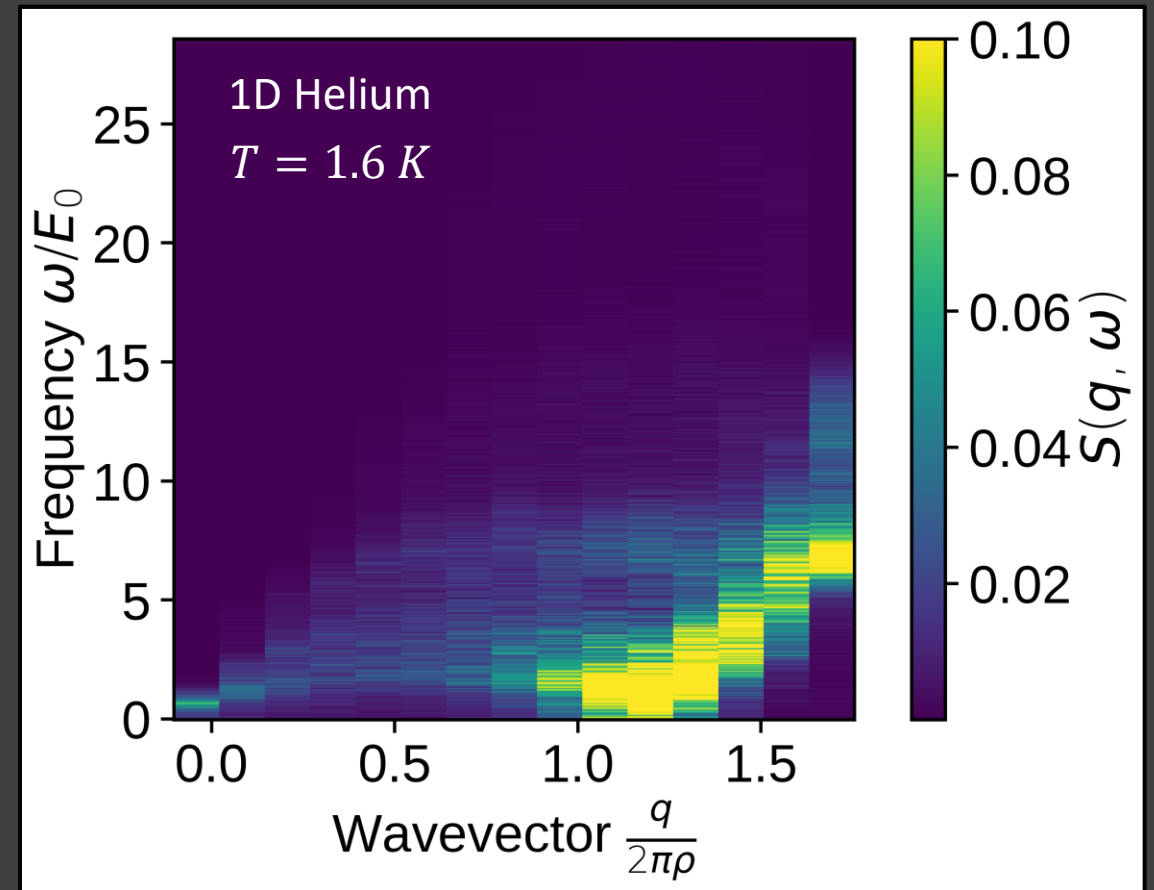


Helium Test Particle Insertion Results



Future Work

- Investigate test particle insertion as function of z
- Molecular dynamics of first adsorbed helium layer
- Dynamic structure factor from QMC data



Collaborators



A. Del Maestro – UTK



P. Sokol – IU



G. Warren – IU



J. Vanegas – UVM



T. Prisk – NIST



The University of Vermont

Questions?

GitHub

nscottnichols

DelMaestroGroup

<https://nathan.nichols.live>

<https://code.delmaestro.org>

