



**Università
degli Studi
di Ferrara**

STATI FLUIDI E SUPERCRITICITÀ IN SISTEMI ALTAMENTE CONFINATI

Relatore

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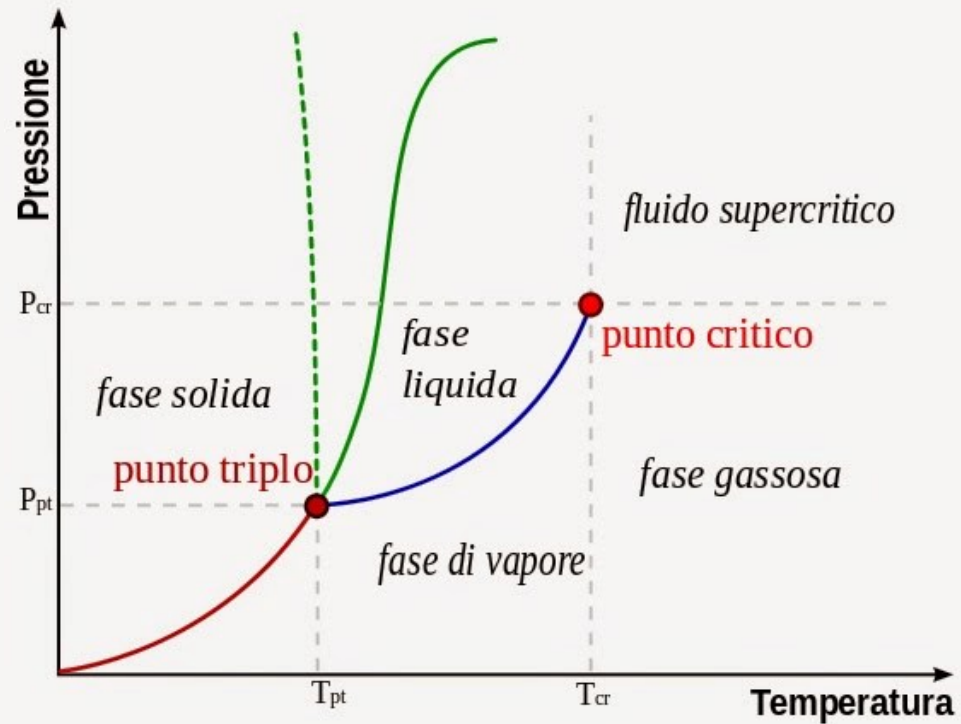
Correlatore

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Laureanda

Marta Alvelli

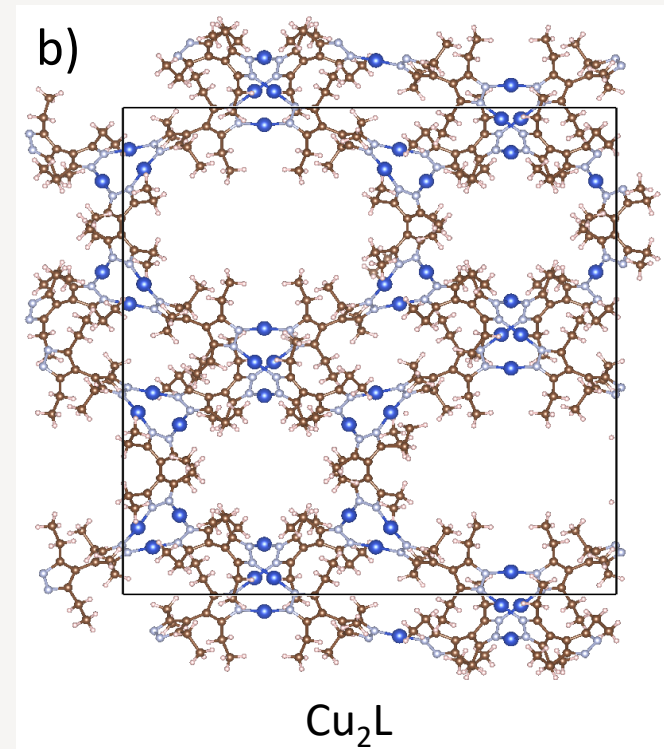
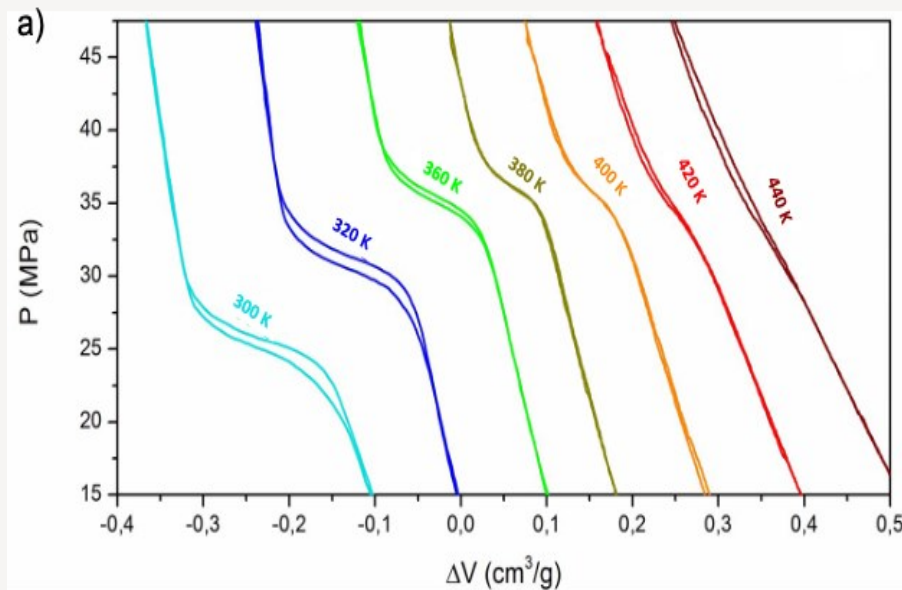
FLUIDI SUPERCRITICI E CONFINAMENTO



Fluidi Supercritici

- Esperimenti di Bernal¹
 - Gas, gas associato | liquido espanso, liquido
- Punto Critico
- Hanno una duplice natura

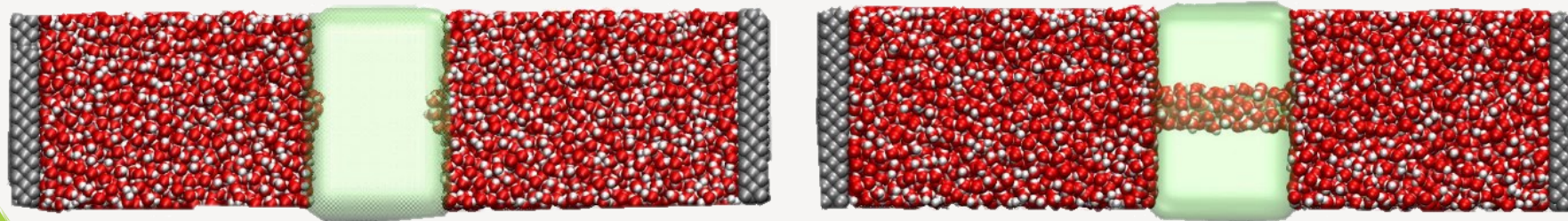
1. J.D. Bernal, Geometric approach to the structure of liquids, Nat. 183 (1959) 141–147. doi: <https://doi.org/10.1038/183141a0>



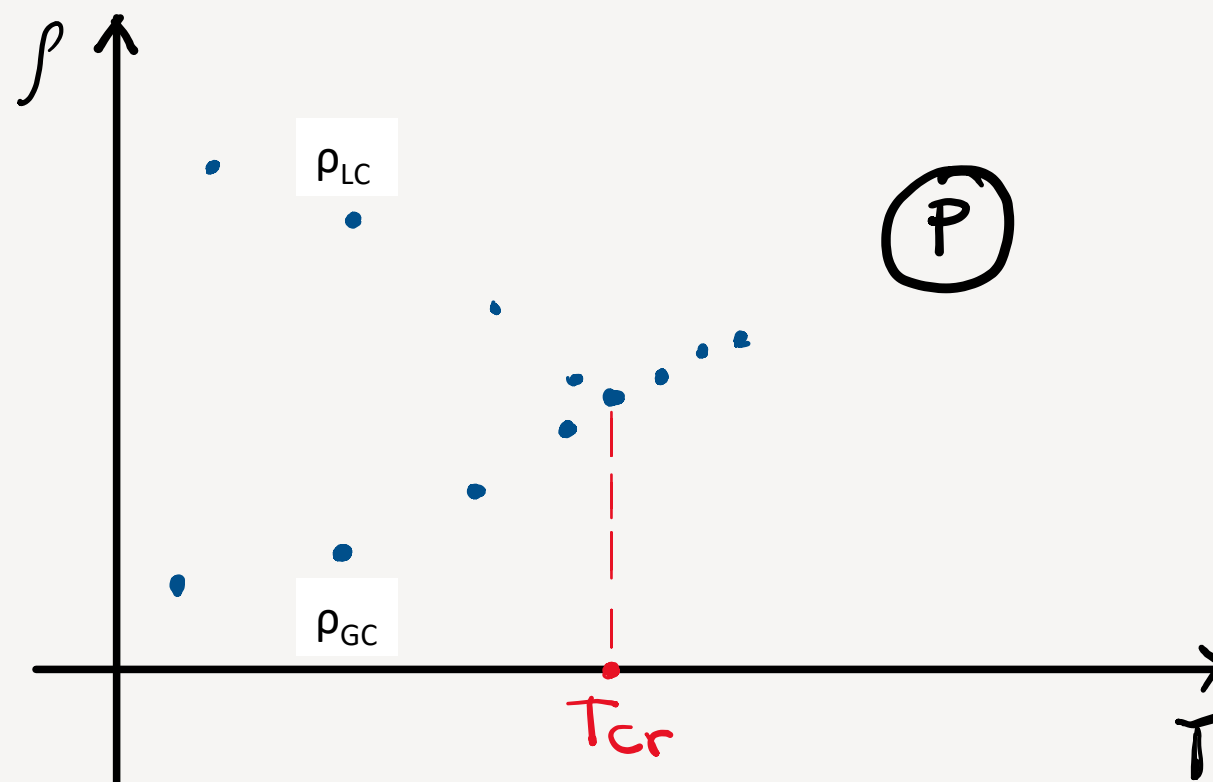
Confinamento

- Mezzi confinanti
 - Può provocare modifiche nella densità, diffusività e le proprietà termodinamiche
- Progetto Europeo FET Electro-Intrusion
- $$V_{int} = \frac{V_{poro}(\rho_{LC} - \rho_{GC})}{\text{number density}}$$

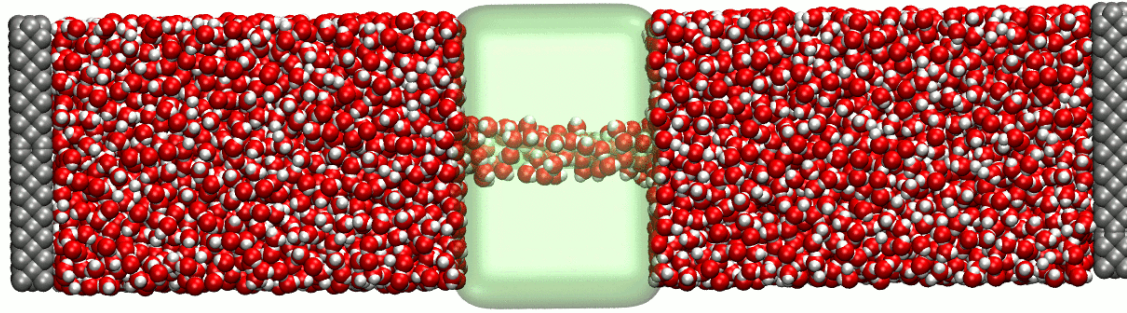
DESCRIZIONE DEL SISTEMA



G. Camisasca, A. Tinti, A. Giacomello, Gas-Induced Drying of Nanopores, J. Phys. Chem. Lett. 2020 11 (21), 9171-9177, doi: 10.1021/acs.jpclett.0c02600



SIMULAZIONI DI DINAMICA MOLECOLARE

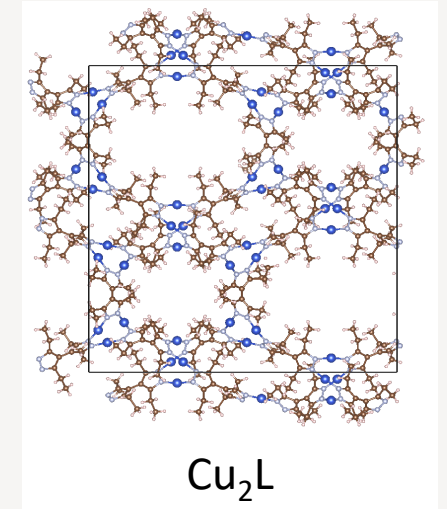
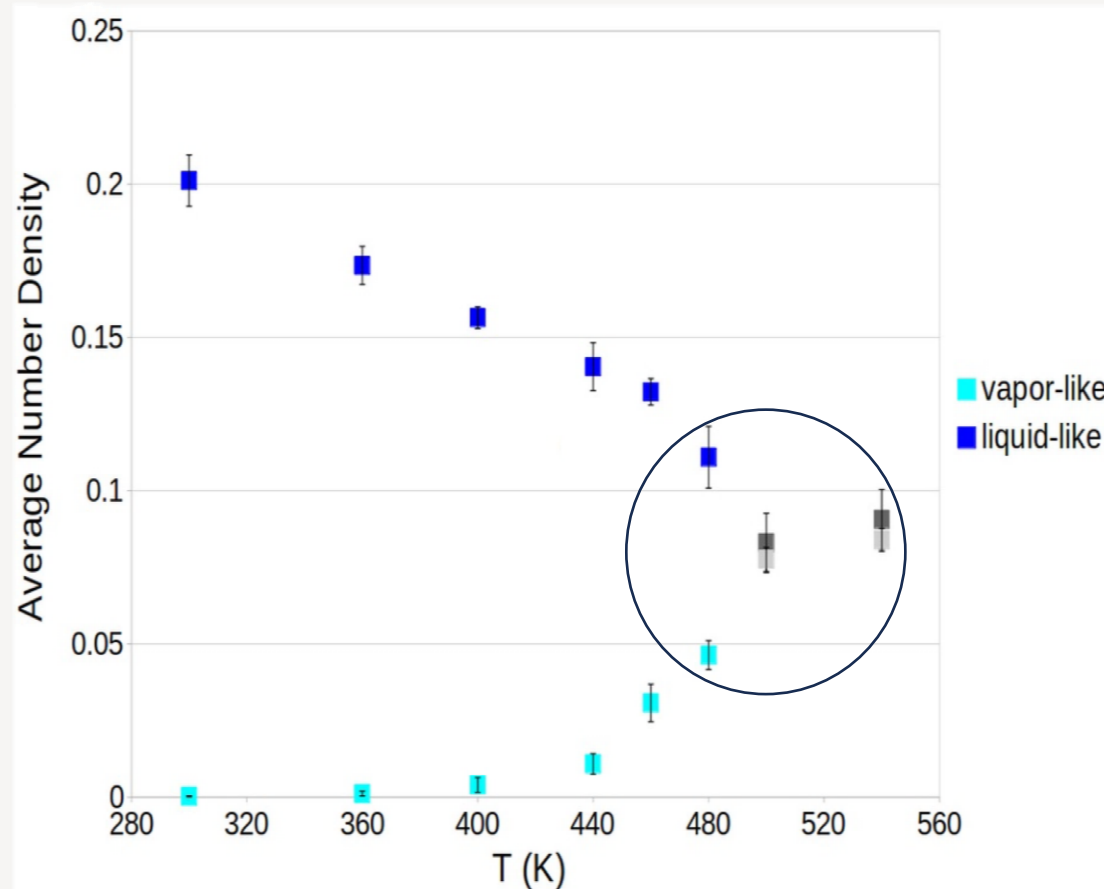


- Pressione esercitata: 20, 25, 30 MPa
- Temperature: 300 K - 650 K con salti di 50 K

Dati Tecnici:

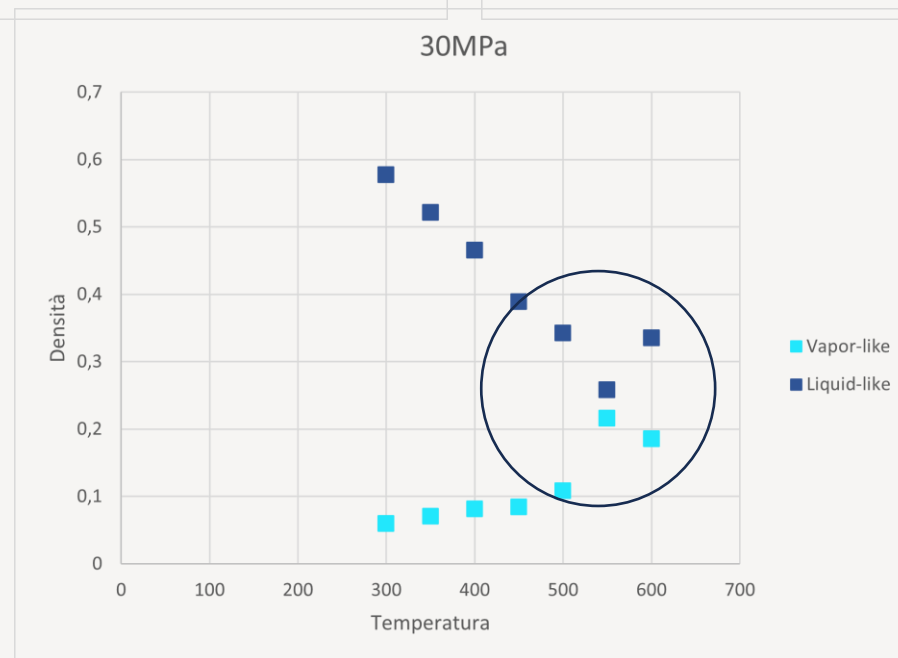
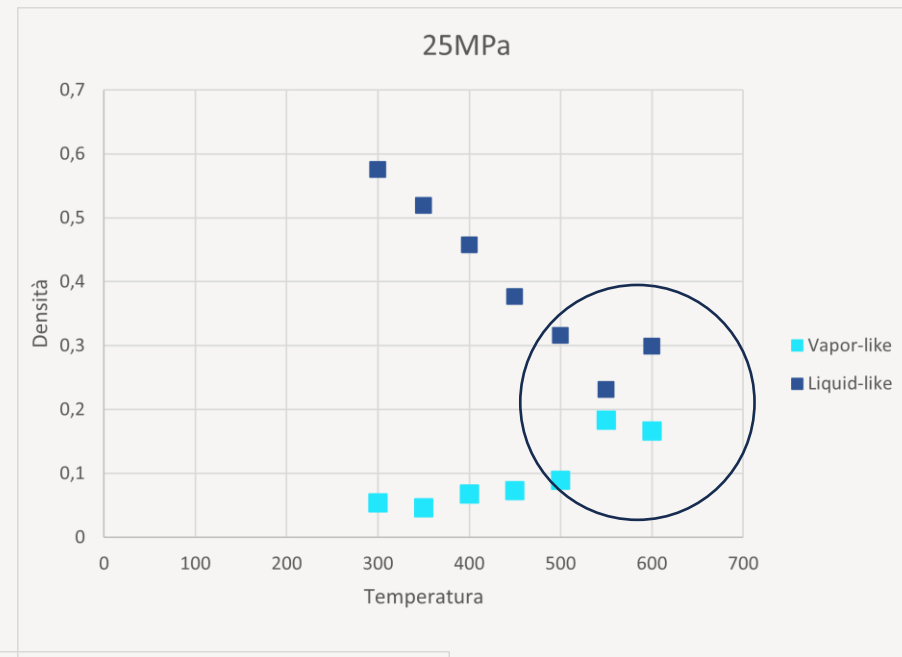
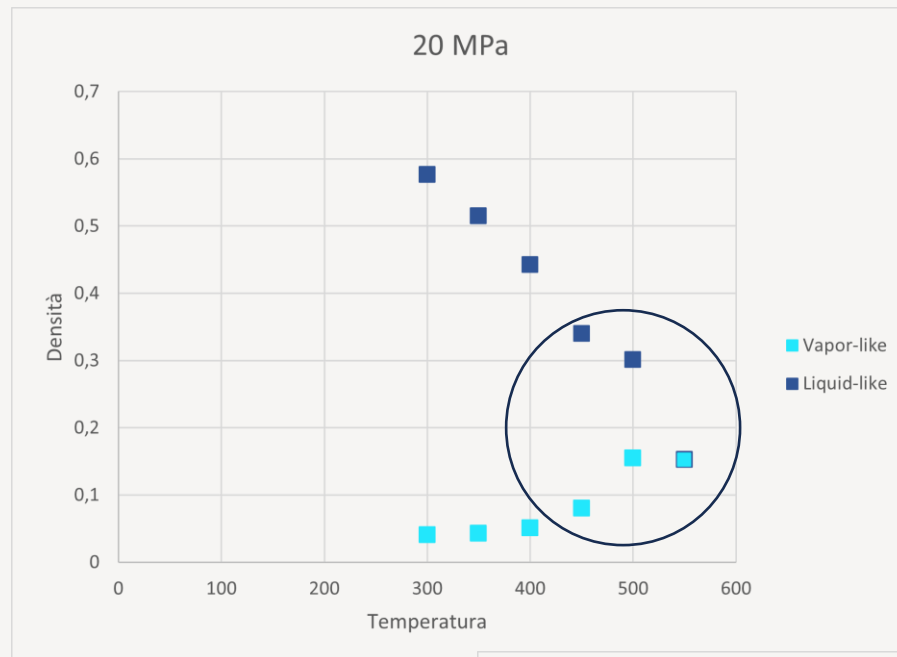
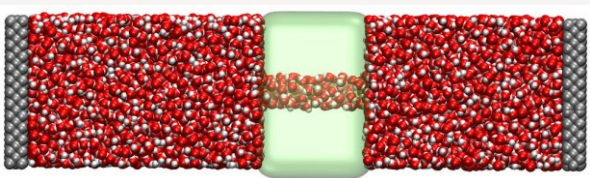
- Intervallo temporale: 1 fs
- Durata simulazioni: 5 ns
- Valore di cutoff: 10.0 Å

RISULTATI



Progetto FET Electro-Intrusion
Si nota come i due stati siano indistinguibili



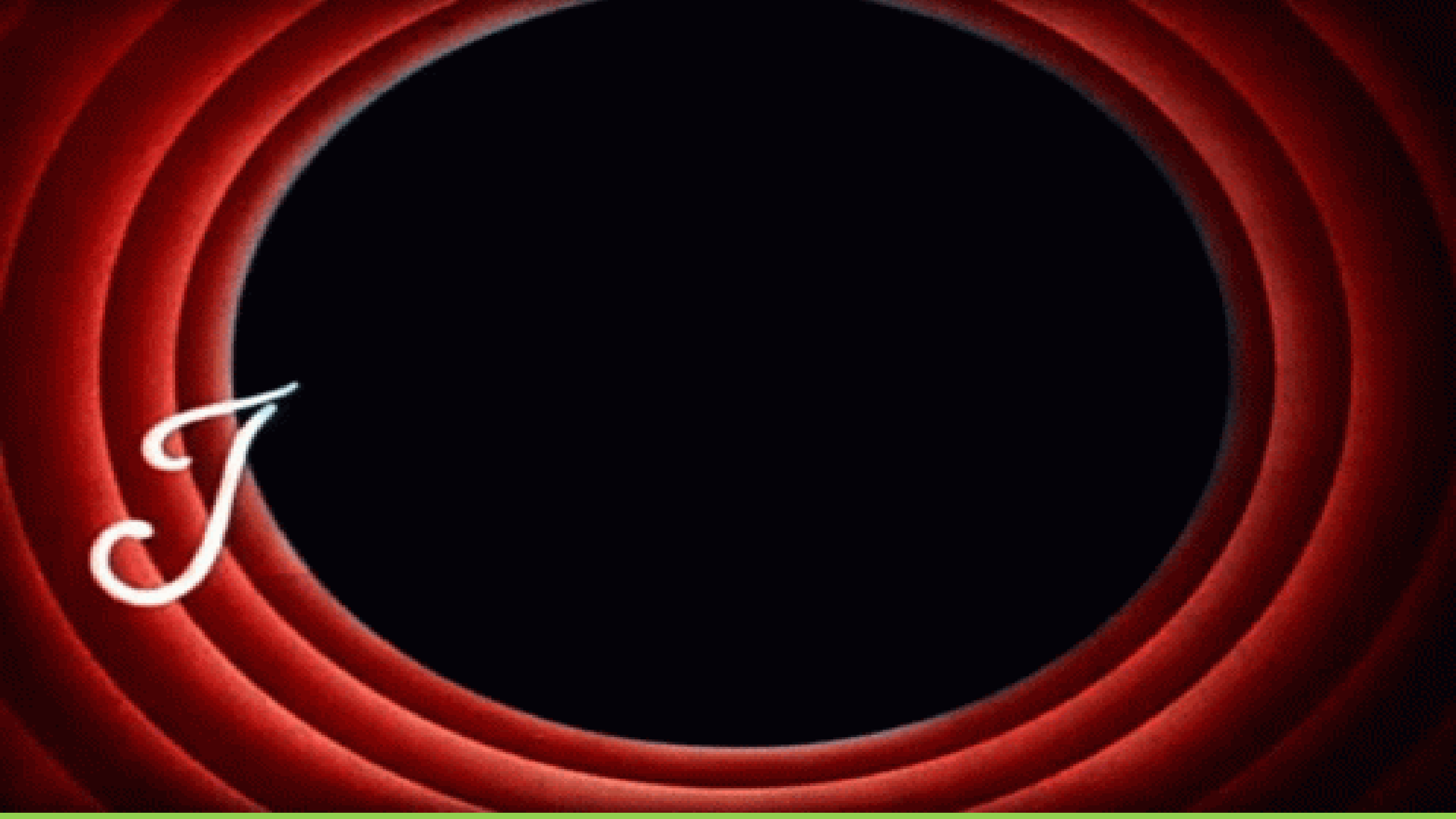


CONCLUSIONI

I risultati sollevano interrogativi sulla natura di questa nuova fenomenologia e richiede ulteriori approfondimenti.

- Sviluppo di nuovi metodi sperimentali e modelli teorici
- Progettazione e realizzazione di nuove strutture di confinamento (i.e. differente larghezza e lunghezza del poro)



The image features a large, stylized white letter 'J' positioned on the left side. The background consists of concentric red circles that create a tunnel-like effect, leading towards a dark blue or black center. The red circles have a slight gradient, giving them a three-dimensional appearance. The overall composition is symmetrical and visually striking due to the high contrast between the white letter, the red circles, and the dark center.

J

- **Hellmann-Feynman**

- $\frac{dE}{d\lambda} = \left\langle \psi_\lambda \left| \frac{d\hat{H}_\lambda}{d\lambda} \right| \psi_\lambda \right\rangle$

- **Forcefield**

- $U = U(R) = \Sigma_{bonds} k_b (r_i - r_0)^2 + \Sigma_{angles} k_a (\theta_i - \theta_0)^2 + \Sigma_{dihedrals} k_\theta [1 + \cos(n_i \Phi_i + \delta_i)] + \Sigma_{impropers} k_\omega (\omega_i - \omega_0)^2 + \Sigma_i \Sigma_{j \neq i} 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \Sigma_i \Sigma_{j \neq i} \left(\frac{q_i q_j}{\varepsilon r_{ij}} \right)$

- **Potenziale di Lennard-Jones**

- $\Sigma_i \Sigma_{j \neq i} 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$

