# CONFINED POLYMERS AS SELF-AVOIDING RANDOM WALKS ON RESTRICTED LATTICES

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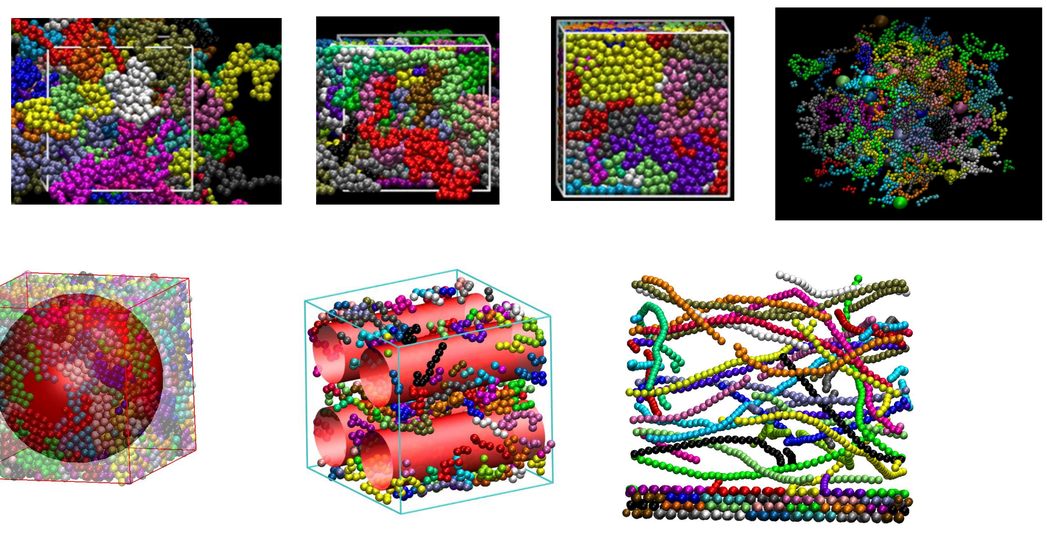
## Motivation

- **Study the effect of extreme confinement** on the **athermal polymer crystallization.**
- **Entropy** is the sole driving force for the **phase transition** of **freely-jointed chains** of tangent **hard spheres**.
- Calculate the configurational entropy of single polymers as by **direct enumeration** of the **self-avoiding random walks** (**SAWs**) on crystal lattices under spatial restrictions imposed by **confinement**.

$$S = k_B ln\Omega$$

## MC simulations under extreme confinement

- Linear, freely-jointed chains of hard spheres of uniform size
- Monte Carlo suite for complex, polymer-based systems [1-3]
- Spatial Confinement: impermeable, parallel flat walls



***Tube-like:***

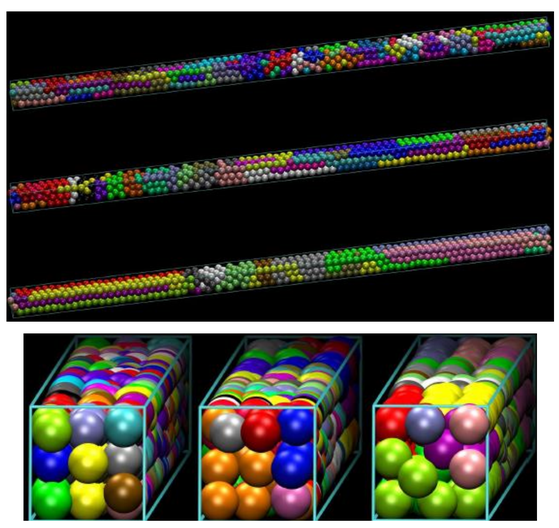
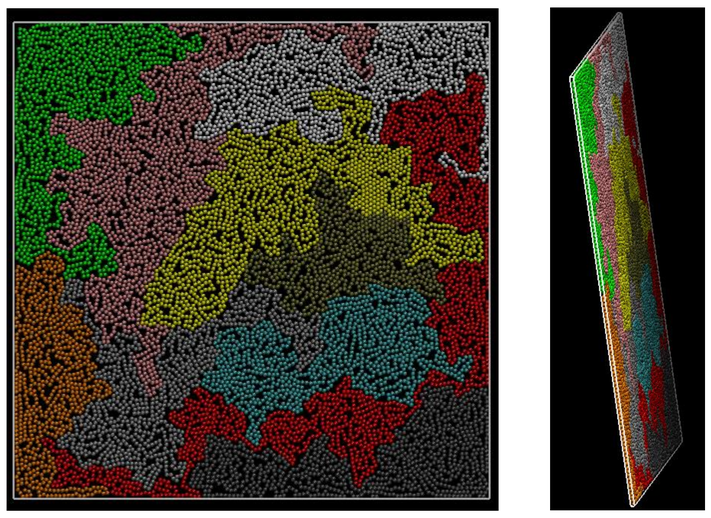
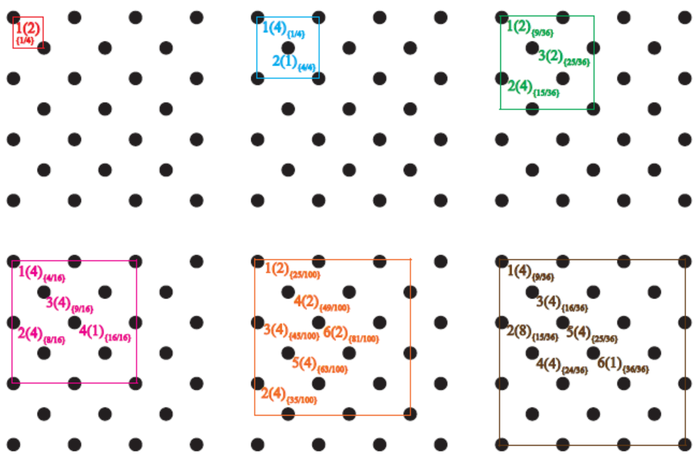


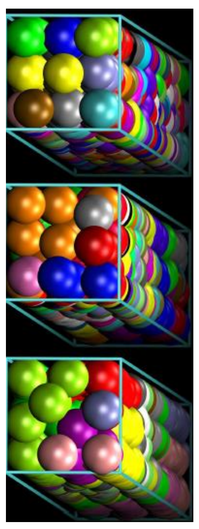
***Plate-like:***



## SAWs in tube-like systems

- New degrees of freedom due to confinement [5]:
  - Tube orientation
  - Tube diameter
  - SAW origin

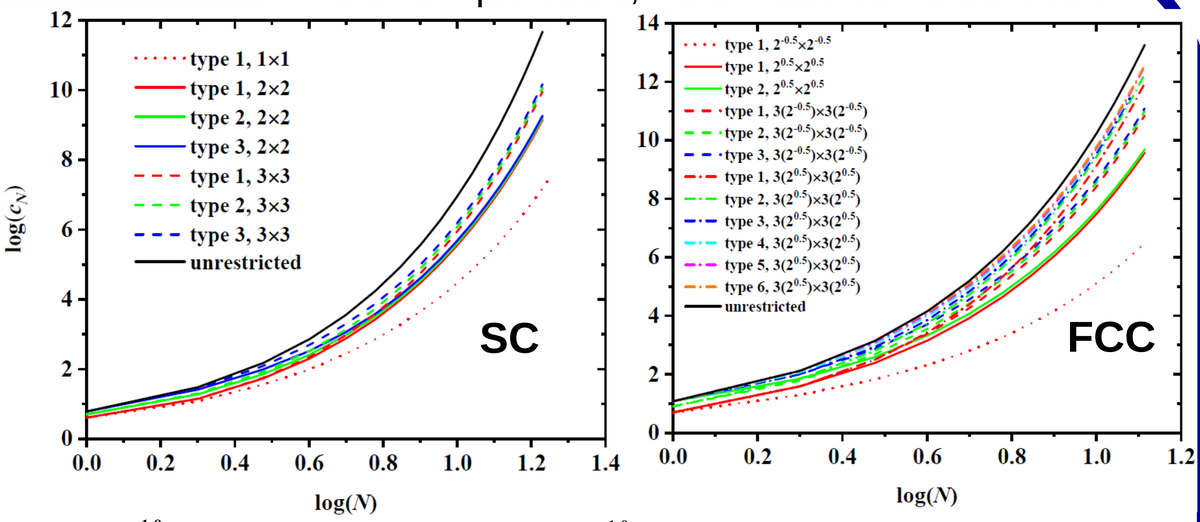


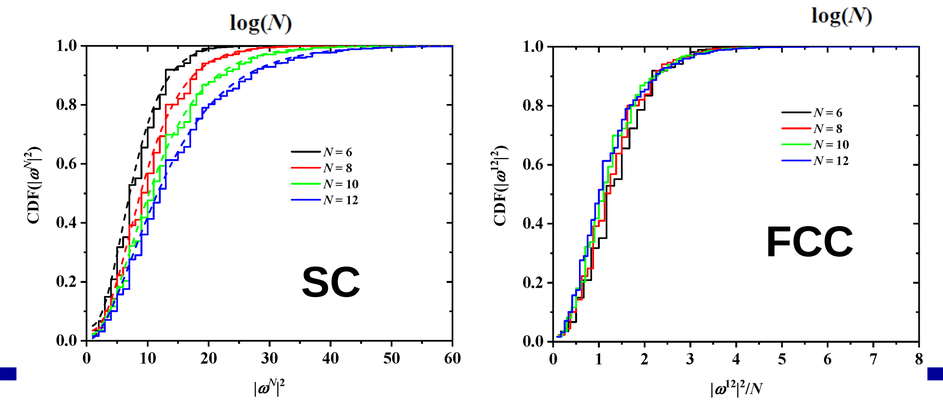


Output

- Number of SAWs $c_N$ : $c_N \sim A\mu^N N^{\gamma-1}$
- Mean-square end-to-end distance : $\langle|\omega^N|^2\rangle \sim DN^{2v}$

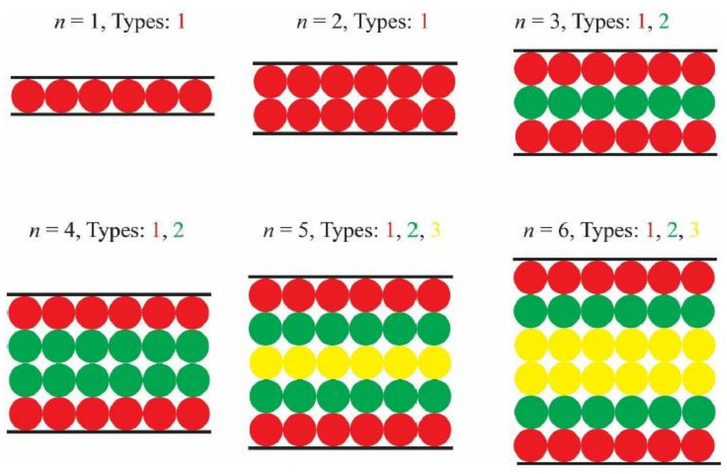
SC: Simple cubic; FCC: Face centered Cubic



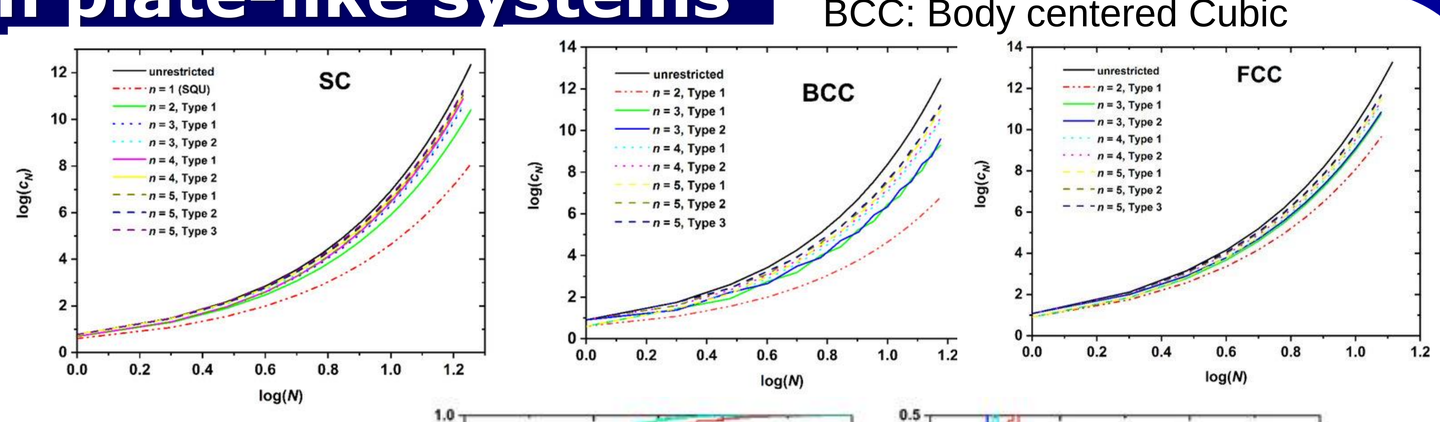



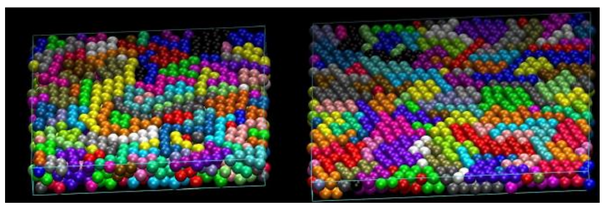

## SAWs in plate-like systems

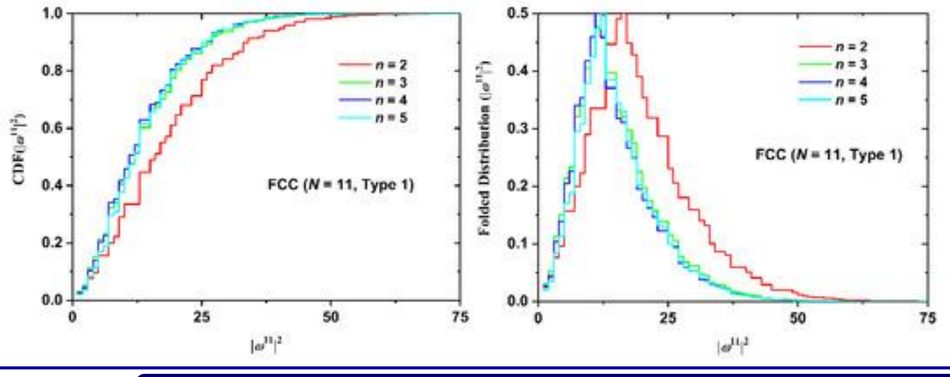
- Types of origin for the enumeration of SAWs for systems under plate-like confinement [6].




BCC: Body centered Cubic






CDF: Cumulative distribution function

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## References

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