Phase Diagram for Single-Patchy-Particles

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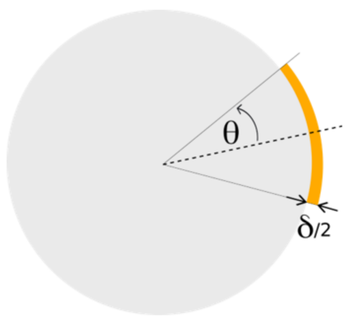
Introduction

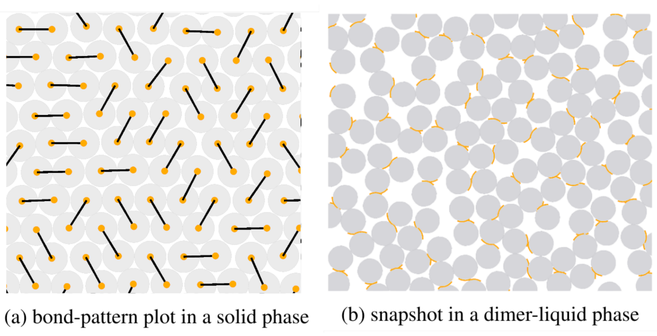
- patchy particles in two dimensions with Kern-Frenkel type potential [1]
- **existing literature:** phase diagrams computed using self-consistent phonon theory (SCP) by [2]
- **simulation approach:** computing regions of coexisting solid and fluid phases using MC simulation techniques
- **theoretical approach:** RTPT-CF [3,4]



$\theta = 27.0°$

$\delta = 0.05\sigma$

Particle Configurations



(a) bond-pattern plot in a solid phase (b) snapshot in a dimer-liquid phase

- **solid**: disks arrange on a hexagonal lattice and form dimer bond patterns
- **fluid**: mixture of dimers and monomers with no positional order

Simulation Details

- NVT-MC and NPT-MC simulations-âĂŃ
- quenching system from high temperatures (hard disk reference state)âĂŃ
- compressing system starting from low pressures (ideal gas reference state)âĂŃ
- $N = 576$ particlesâĂŃ
- 1e6âĂŃ cycles

[1] N. Kern, D. Frenkel, J. Chem. Phys., 118, 9882 (2003)

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[4] Y. V. Kalyuzhnyi, H. Docherty, P. T. Cummings, J. Chem. Phys. 135, 014501 (2011)

[5] C. Vega, E.G. Noya, J. Chem. Phys. 127, 154113 (2007)

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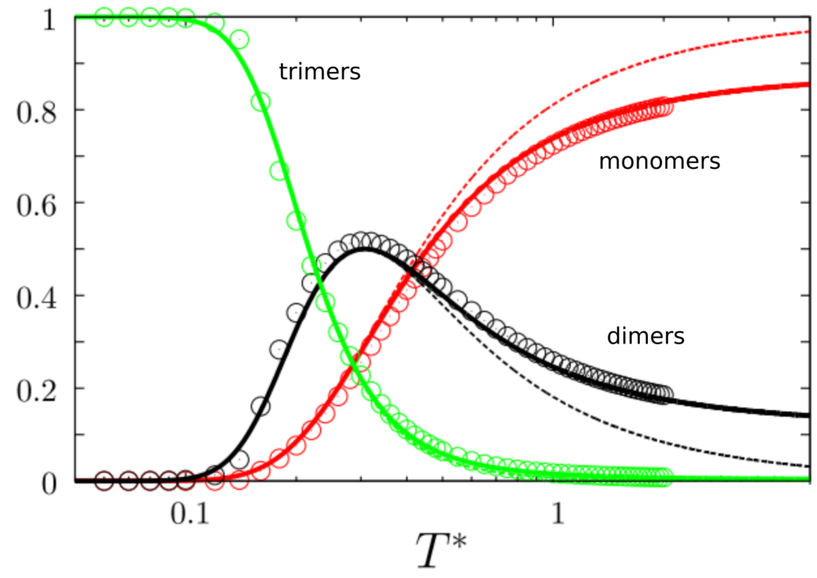
Theory and Simulation Comparison

- results from the theoretical framework **multidensity resummed thermodynamic perturbation theory for fluids with central-force type of associative potential (RTPT-CF)** [3,4] are depicted in solid lines for particles with $\theta = 43°$ and $\delta = 0.5\sigma$
- simulation results in circles



From Thermodynamic Integration To Coexistence

- **Einstein Molecule Method** [5] is applied to compute Free Energy of hard disks
- **solid:** thermodynamic integration along isochors with hard disk FE ($\beta = 0$) as reference system:

$$A(\rho, \beta_2)[Nk_BT] = A(\rho, \beta_1)[Nk_BT] + \int_{\beta_1}^{\beta_2} \frac{U(\rho, \beta)}{N} d\beta$$

- **fluid:** thermodynamic integration along isotherms with ideal gas as reference system:

$$A(\rho_2, T)[Nk_BT] = A(\rho_1, T)[Nk_BT] + \int_{\rho_1}^{\rho_2} \frac{p(\rho, T)}{k_BT\rho^2} d\rho$$

- via the **double tangent construction** the coexistence points are determined.