

Self-assembling of core-corona particles

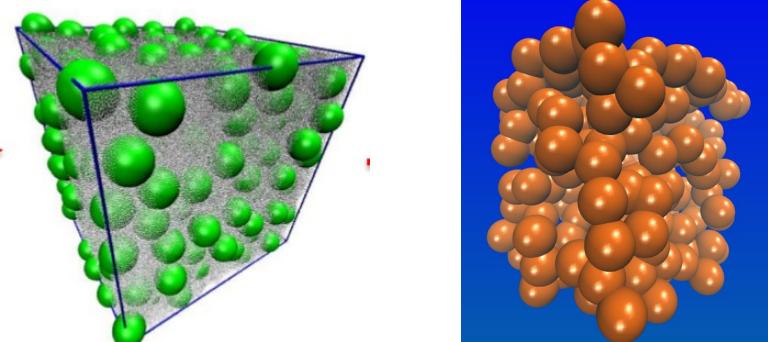
Dr. Gabriel Oscar Ibañez-Garcia
UNAM, Campus Juriquilla
Septiembre de 2022.





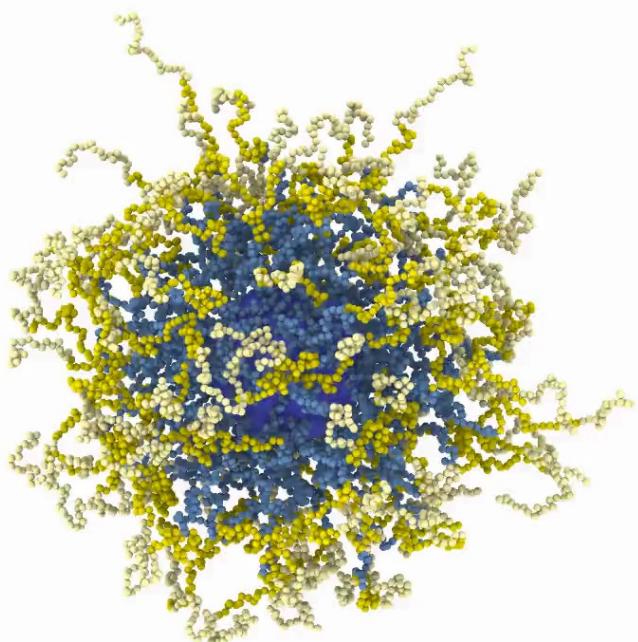
Colloidal particles

- Spherical particles of diameter:
10 nm-1micron
- Immersed in liquid
- Colloidal Suspension
- Brownian Motion

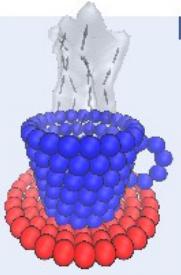




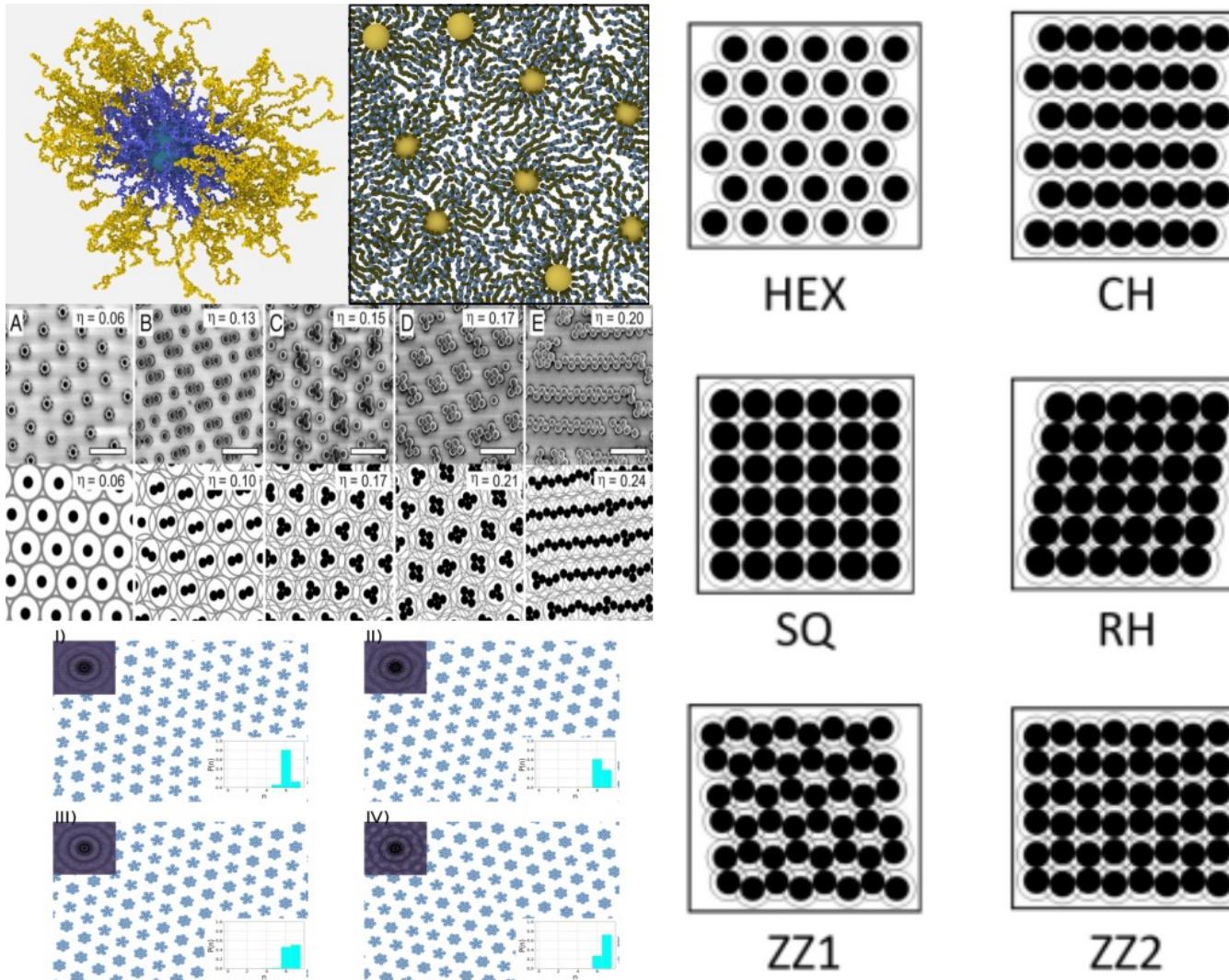
Core Corona particles



- Colloidal particles covered with polymer ligands.
- Size 100nm a 1micra.
- Corona is equal or longer than the core diameter.
- Purely repulsive Interations

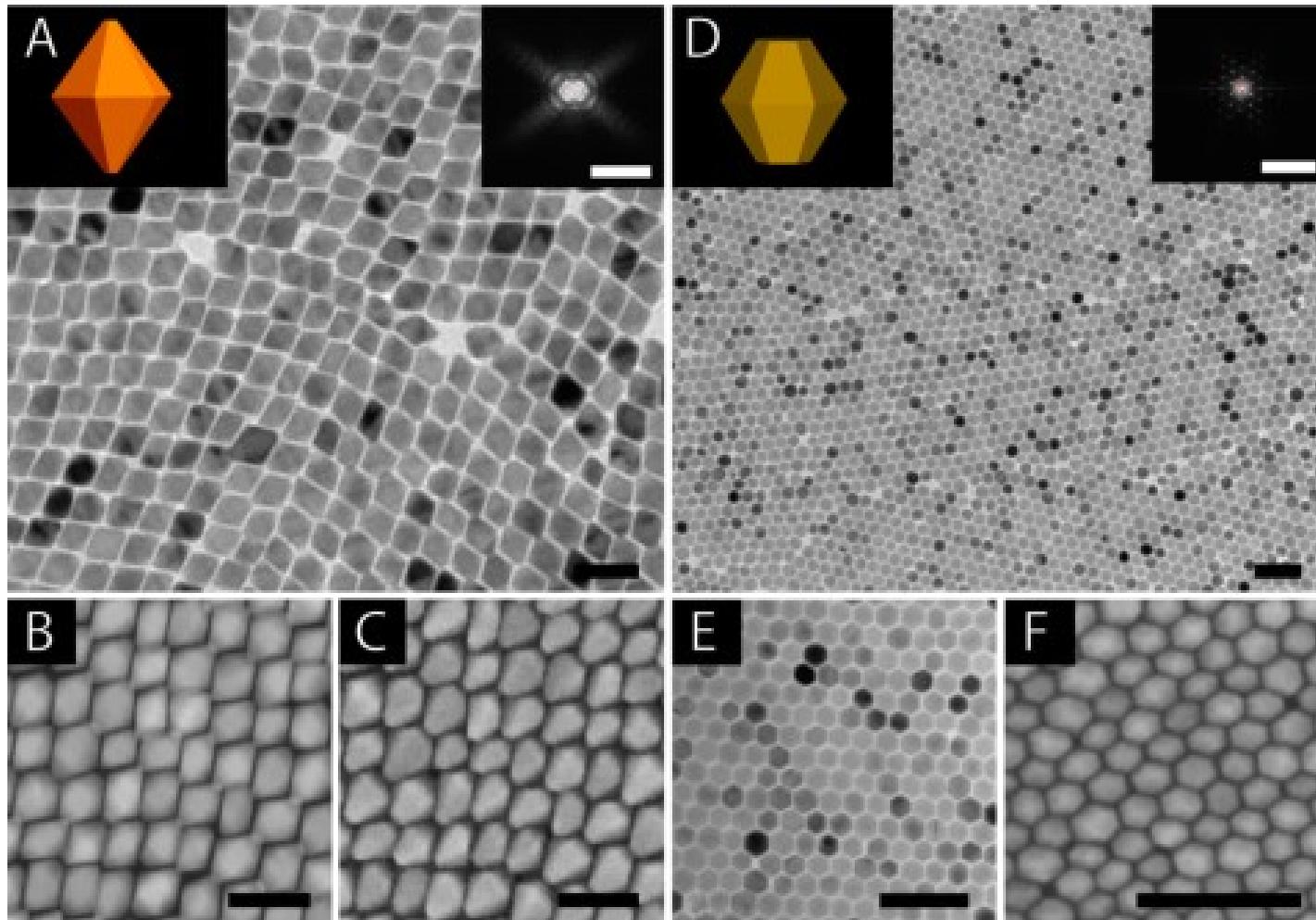


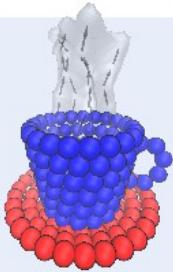
Self-Assembling: purely repulsive interactions





Self-Assembling: purely repulsive interactions

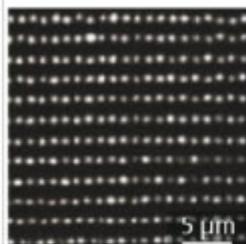




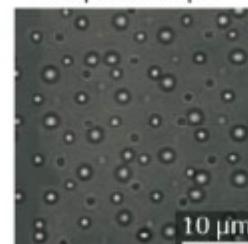
Self-Assembling:mechanisms

External field

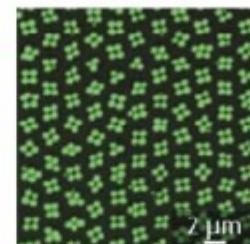
a Electric field



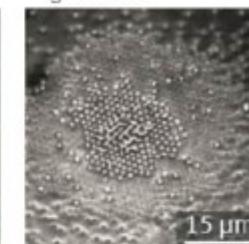
b 3D quasicrystals in optical traps



c Magnetic traps on substrates

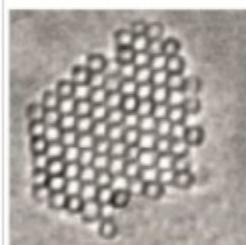


d Temperature gradient

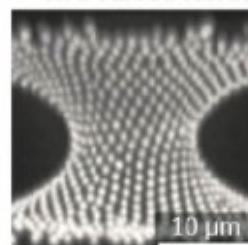


Liquid solution

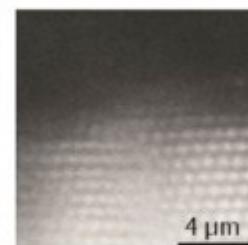
e Depletion



f Capillary attraction on a curved surface

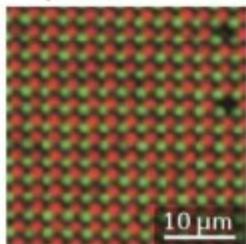


g Casimir-like attraction

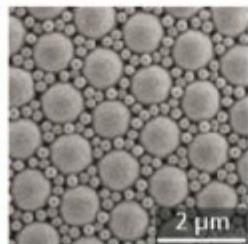


Bidisperse colloids

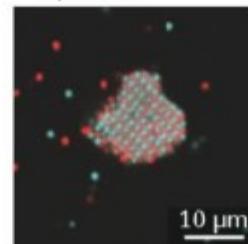
h +/- charged spheres



i Big/small spheres

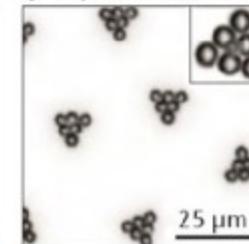


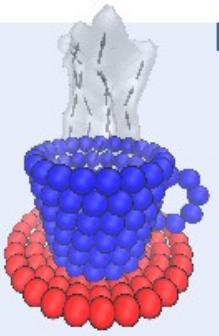
j DNA-coated spheres



Competing interactions

k Capillary, dipolar and hydrophobic interactions



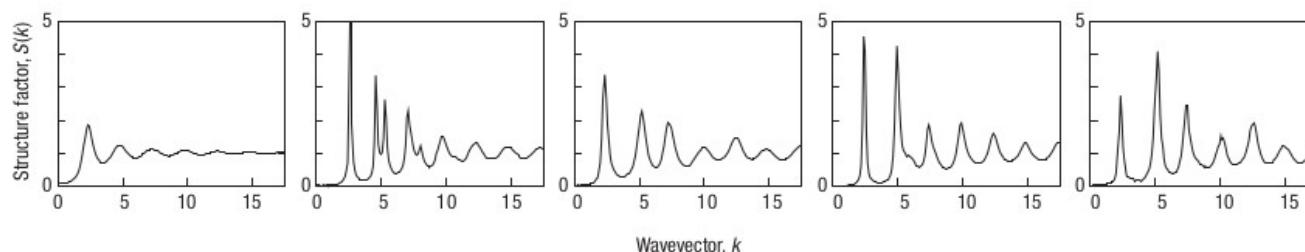
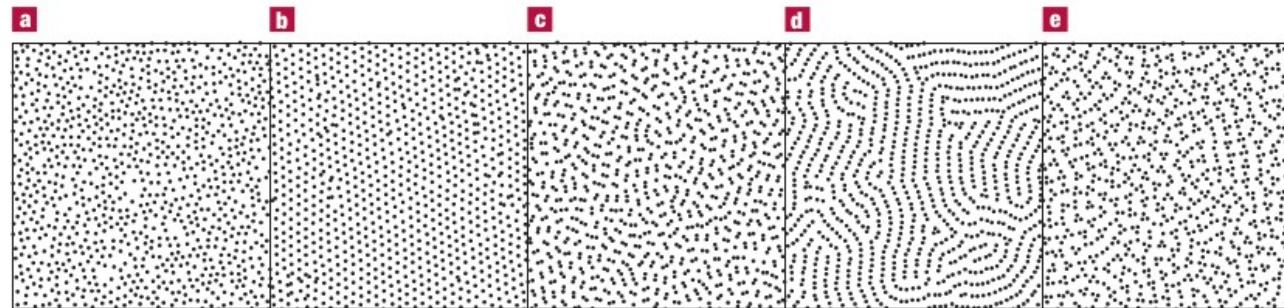
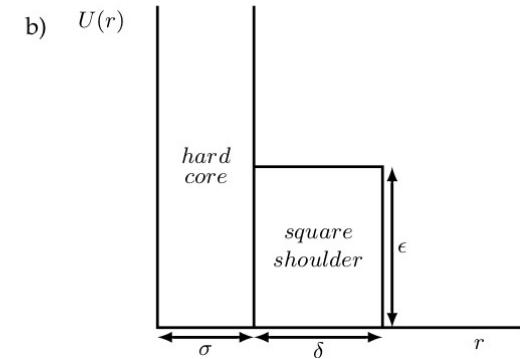
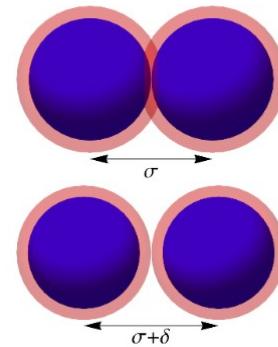


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Core Corona Particles

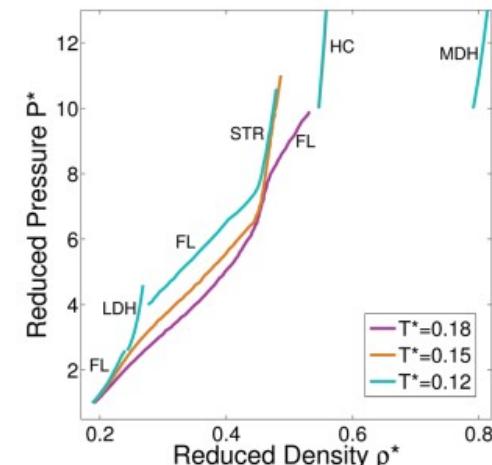
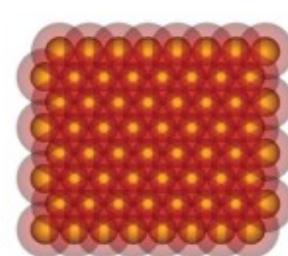
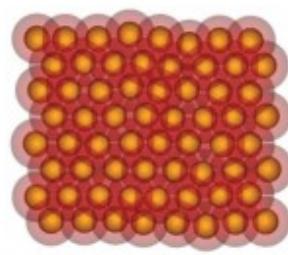
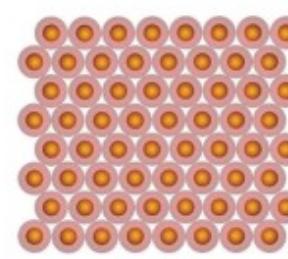
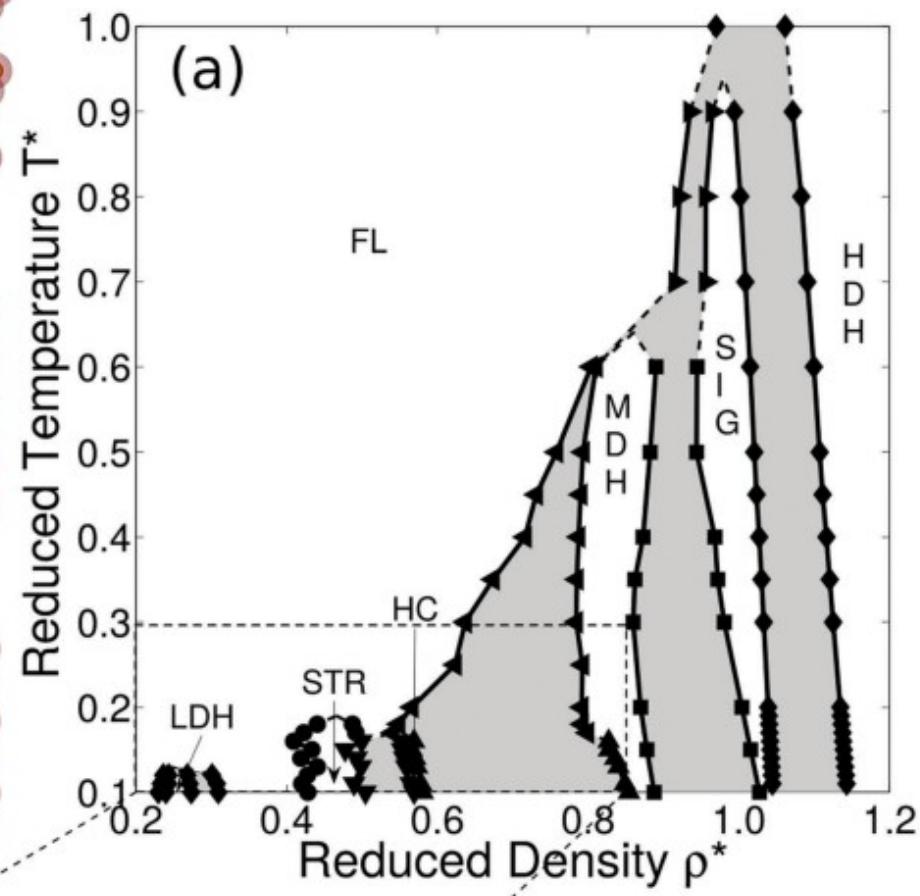
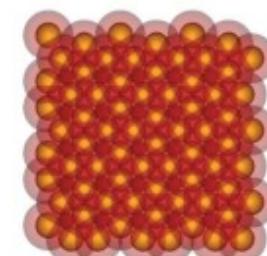
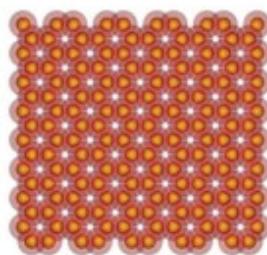
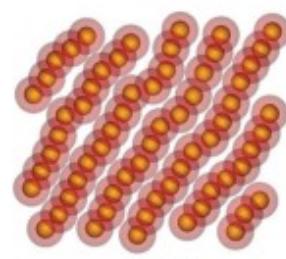
Hard Core Square Shoulder model

$$U(r) = \begin{cases} \infty, & r < \sigma, \\ \epsilon, & \sigma < r < \sigma + \delta, \\ 0, & r > \sigma + \delta, \end{cases}$$



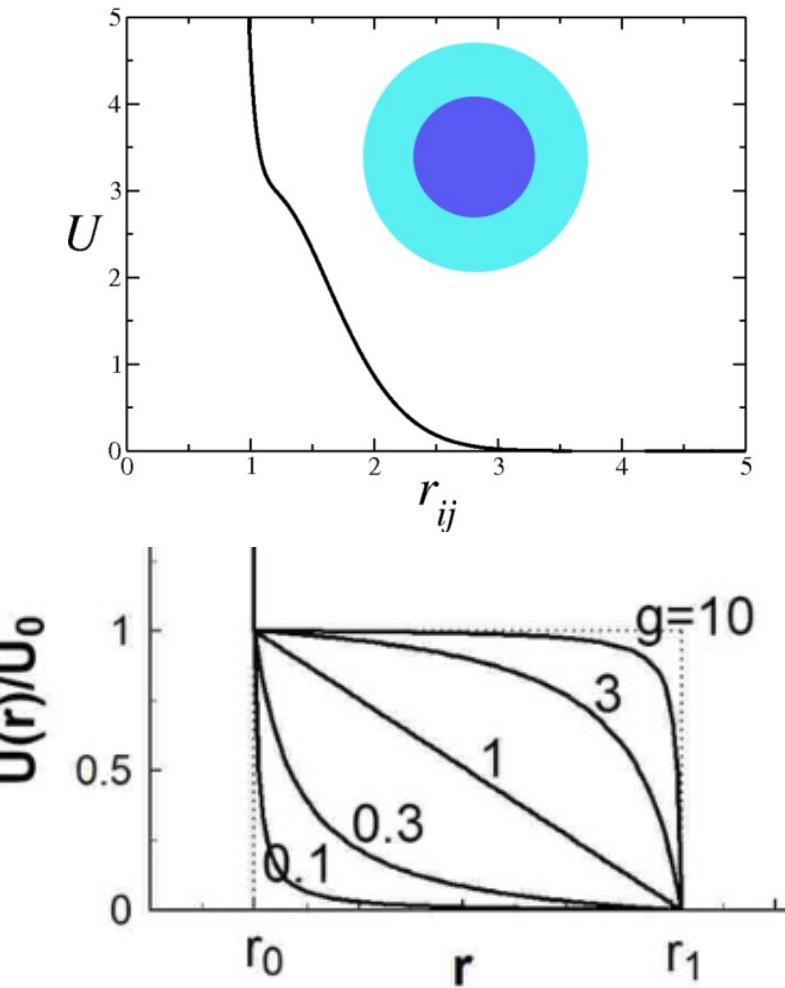


Different mesophases

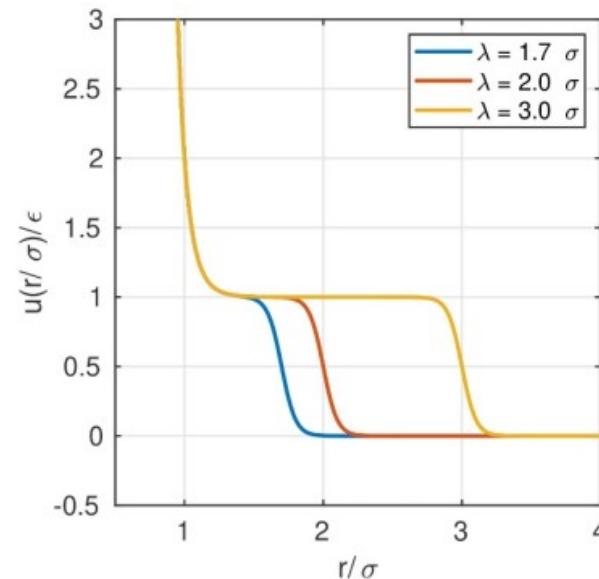


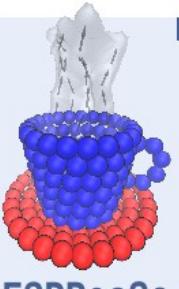


Another Core-Corona models



- 1.-Classical square-shoulder (Ideal model)
- 2.-Gaussian + Lennard Jones
- 3.-Hyperbolic tangent
- 4.-Linear and Spline model





Models for core-corona particles

Truskett [1]: Liquid → Hexagonal → Square → Pairs → String → Kagome → Hexagonal

Torquato [2]: Liquid → Hexagonal → String → Kagome → Hexagonal

Hertzian [5]: Liquid → Hexagonal → Square → Pentagonal → Stretched Hexagonal → Hexagonal → Square → Rhombohedral → Stretched Hexagonal → Hexagonal

LJY [6]: Liquid → Hexagonal → String → Hexagonal → Kagome → Hexagonal

Core-Corona ($\frac{\delta}{\sigma} = 1.95$) [3]: Liquid → Hexagonal → Liquid → String → Honeycomb → Hexagonal → Sigma → Hexagonal

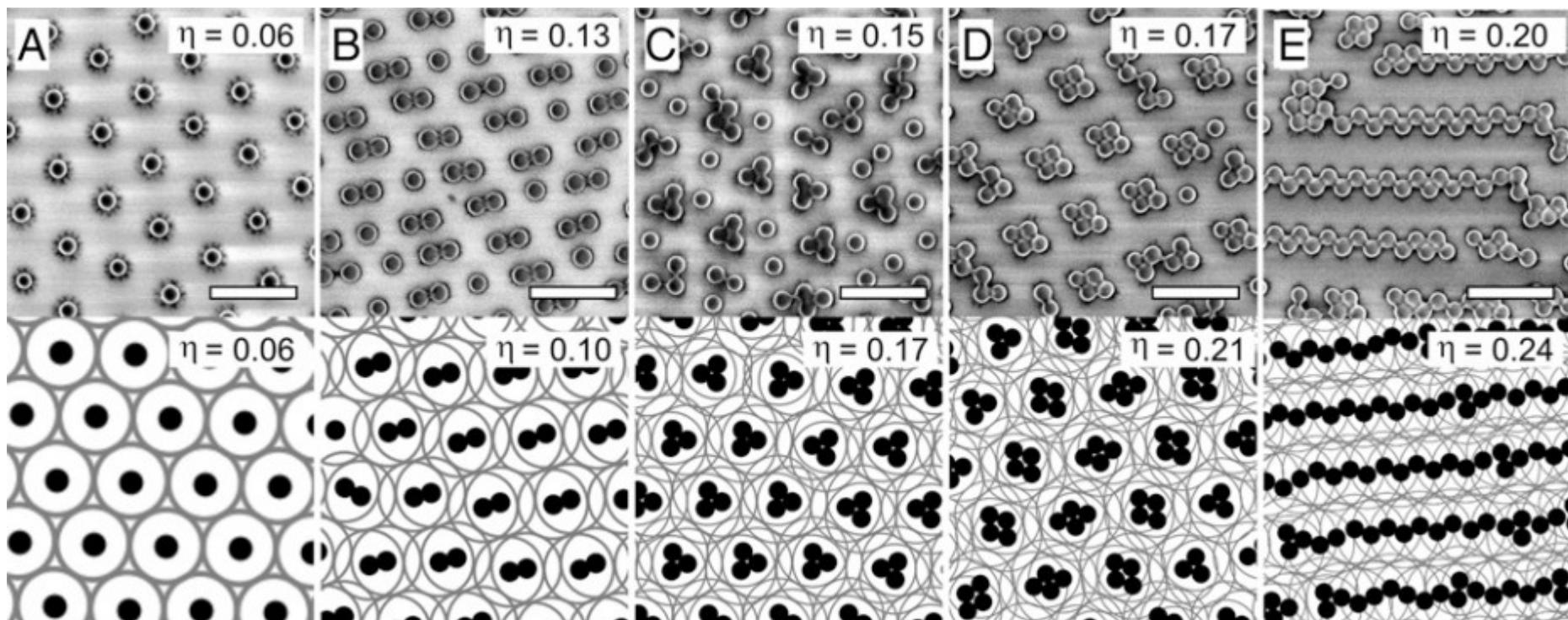
Core-Corona ($\frac{\delta}{\sigma} = 1.40$) [3]: Liquid → Hexagonal → Liquid → Square → Quasi-crystal → Hexagonal

Core-Corona ($\frac{\delta}{\sigma} = 1.27$) [3]: Liquid → Hexagonal → Liquid → Rhombus → Quasi-crystal → Hexagonal

Daoud–Cotton ($f = 50, 68, 150$) [7]: Hexagonal → Stripe → Honeycomb → Kagome → Hexagonal

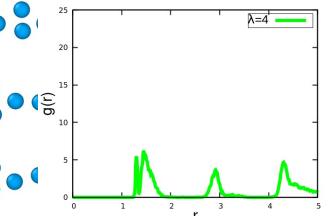
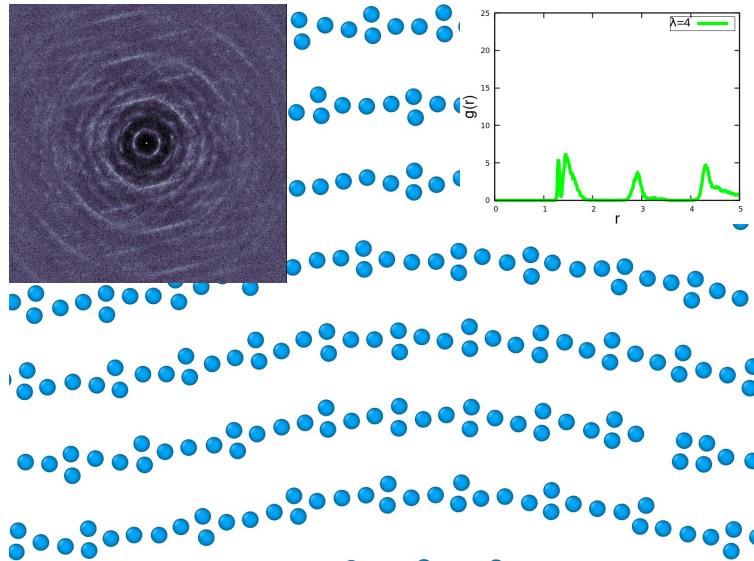
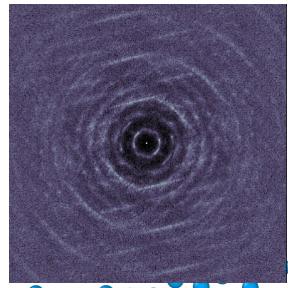
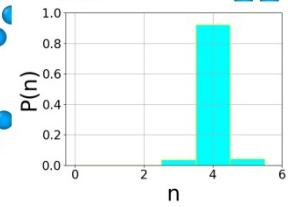
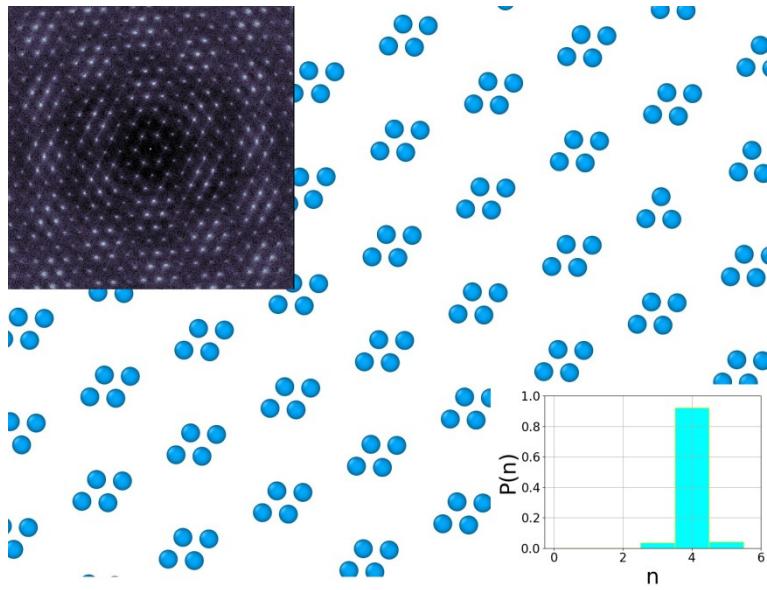
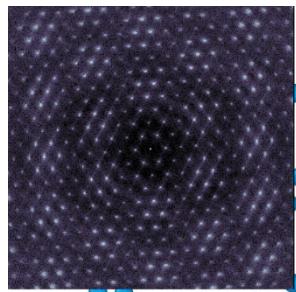
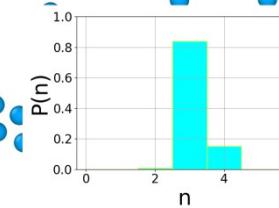
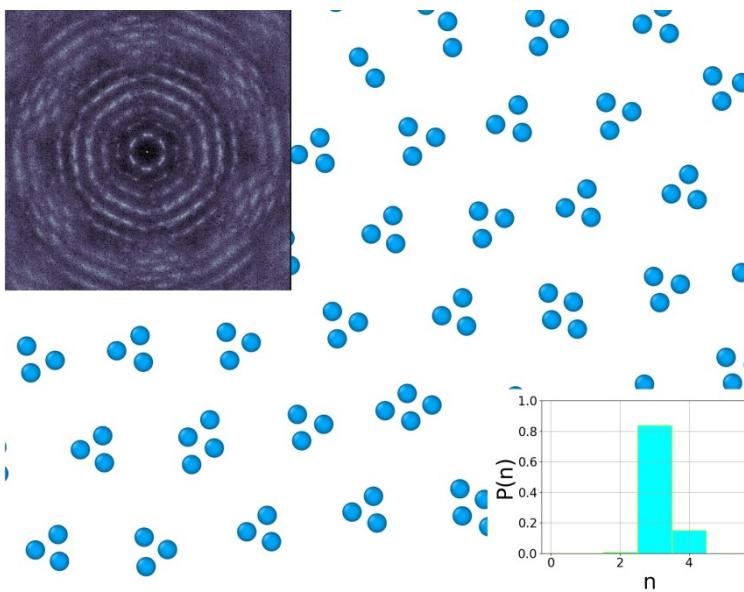
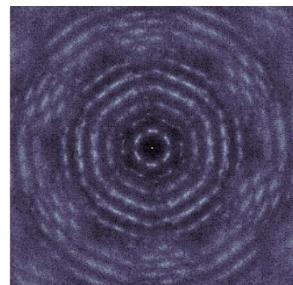


Core-corona clusters: long coronas



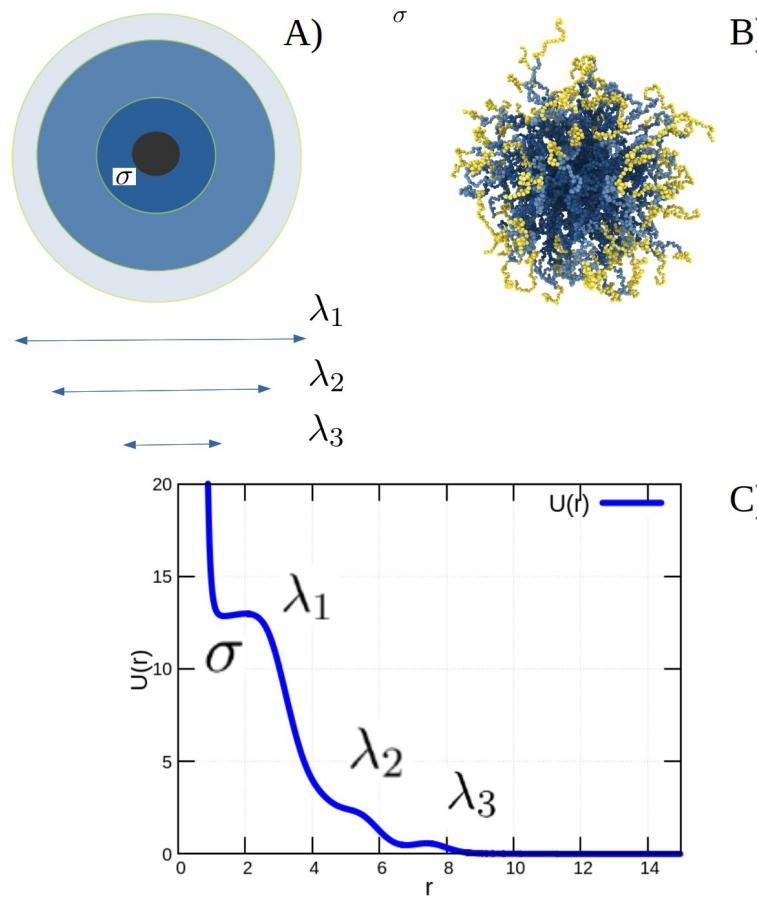


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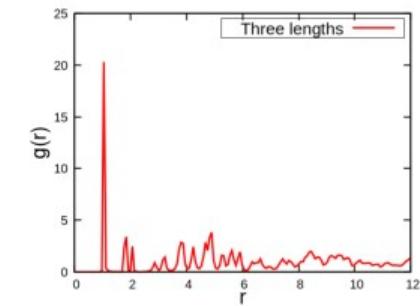
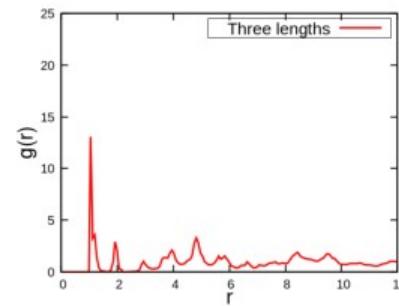
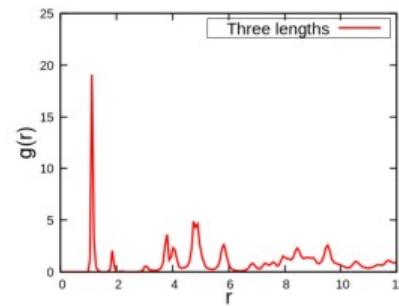
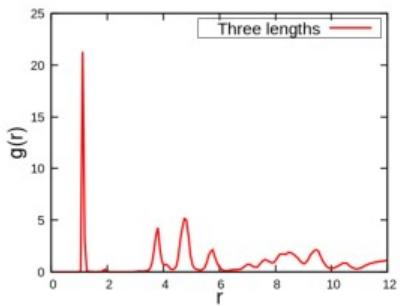
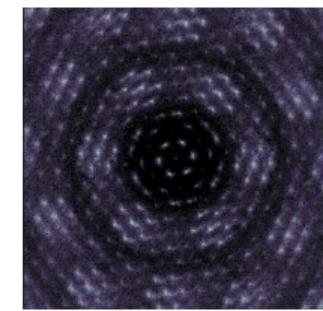
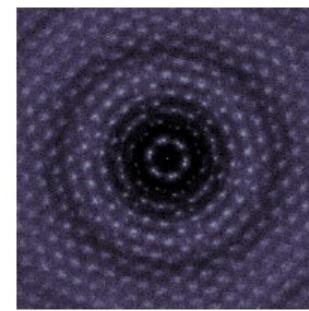
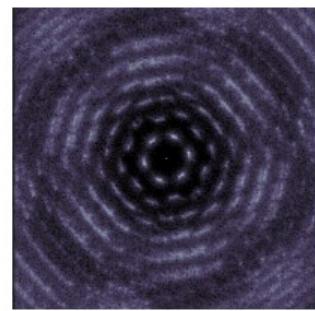
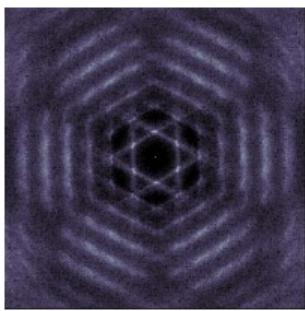
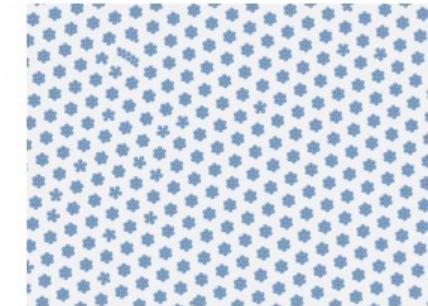
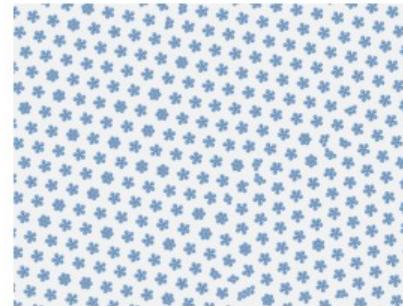
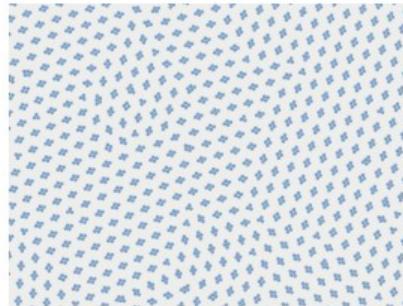
Core-corona clusters : long coronas



$$U(r_{ij}) = \epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} + \sum_{k=1}^M U_k [1 - \tanh((b_k r_{ij} - \lambda_k))] + u_k \exp(-A_k (r_{ij} - r_k)^2) \right]$$

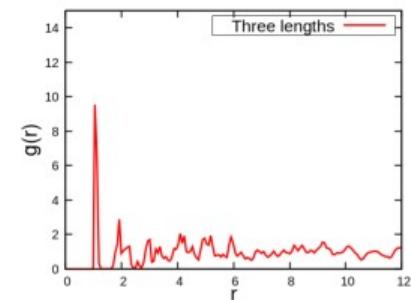
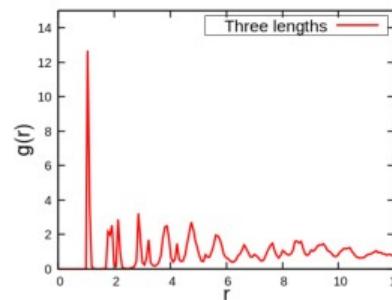
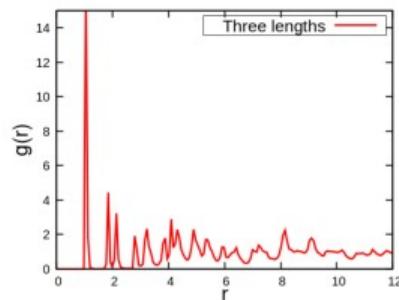
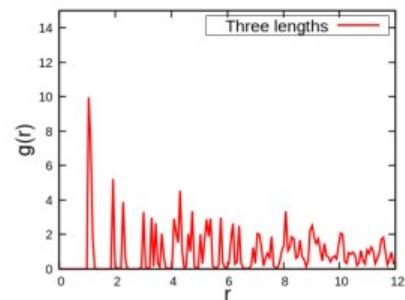
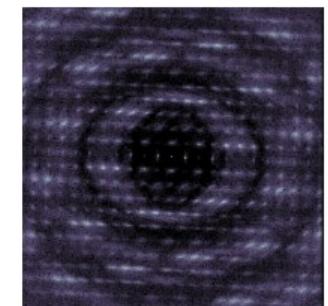
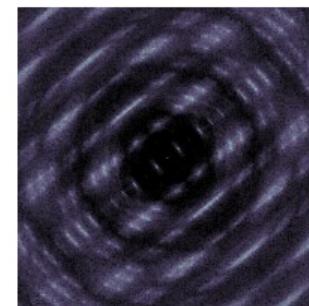
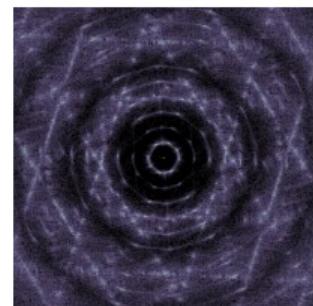
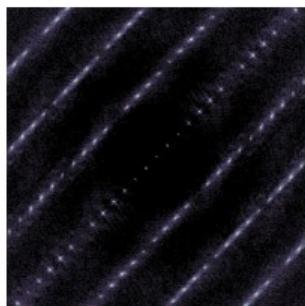
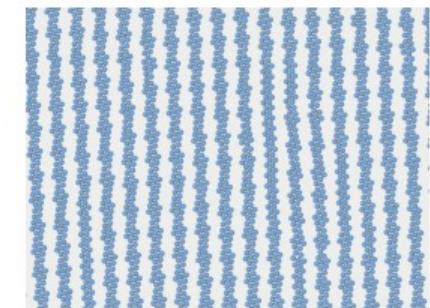


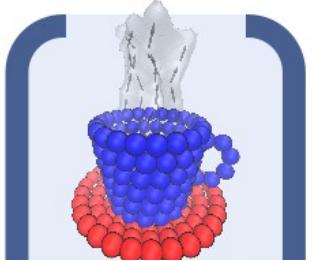
Superlattices de Clusters (core-corona)



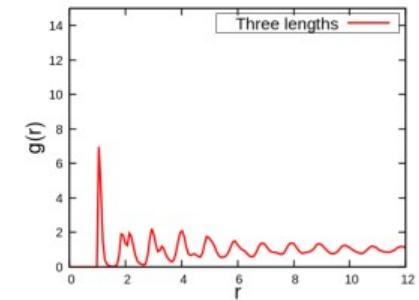
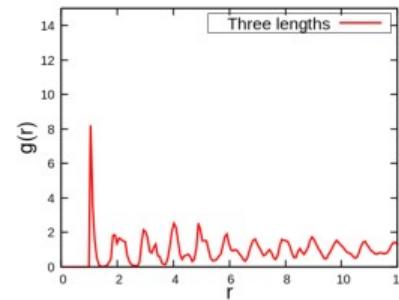
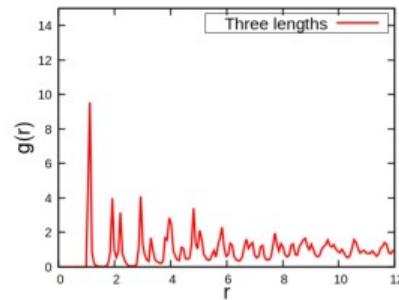
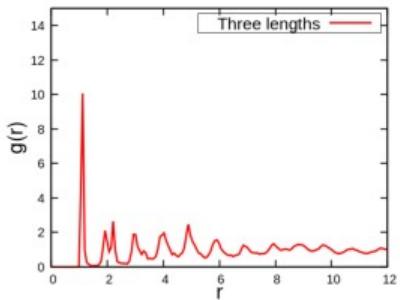
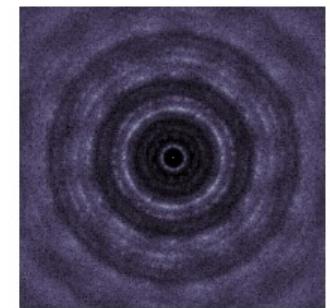
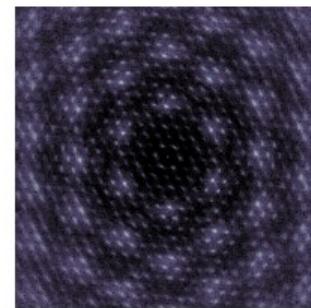
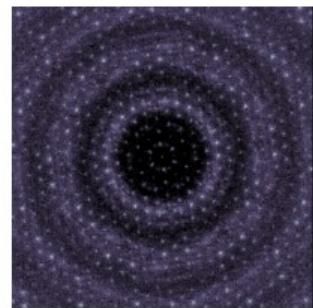
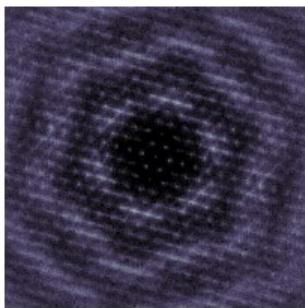
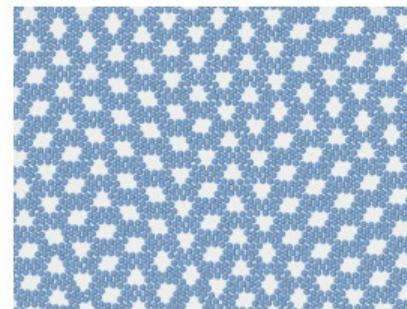


Complex Stripes (core-corona)





Void Networks (core-corona)





Crystal (core-corona)

