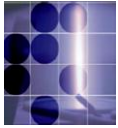


BIOACTER-related topics



Jure Dobnikar

University of Cambridge, UK
Jožef Stefan Institute, Ljubljana, Slovenia



KITP, UC Santa Barbara, January 17th 2014

Modeling bacterial motility

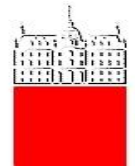
- Fluctuation-induced superdiffusive behaviour in *E. Coli* chemotaxis (*BiophysJ* 2009, *PLoS One* 2011)
- Sensing vs communicating: pattern formation (*PLoS One* 2013)
- Twitching motility in *P. Aeruginosa*: effect of pili microscopic properties (e.g. elasticity) on macroscopic trajectories (*preprint*)

Modeling active colloids

- Walking DNA-coated colloids (*submitted*)
- Phase separation in hard colloids with density-dependent propulsion (*in progress*)
- Interactions between passive colloids induced by active medium (*in progress*)

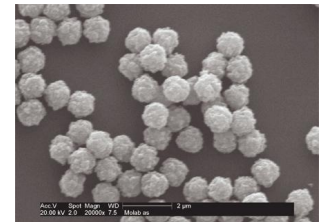
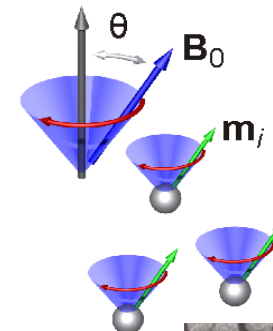
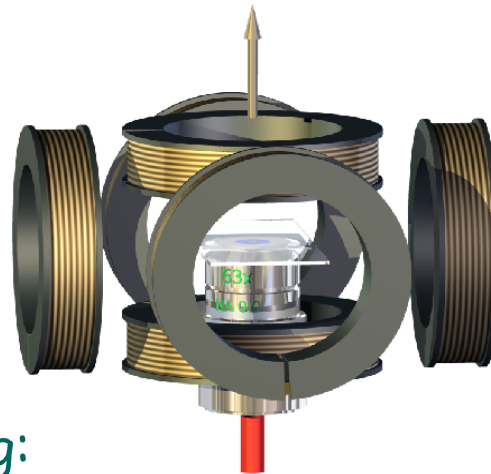
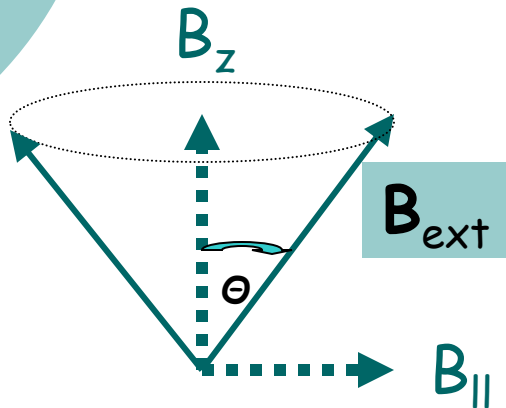
"Almost active" magnetic colloids

EXPERIMENTS: Natan Osterman, Gašper Kokot, Dušan Babič
University of Ljubljana, Slovenia



Superparamagnetic colloids in external time-dependent fields

- Interactions are externally induced
- Driving is the same for all the particles \rightarrow not active
- **Many-body effects**: interactions depend strongly on local structure
- We observe **chains** and **membrane** formation as well as **dynamic vortices**



Dynabeads MyOne, 1 μm

precessing field cone opening:
 $\text{tg}(\Theta) = B_{||}/B_z$

Magnetic interaction: SCFI

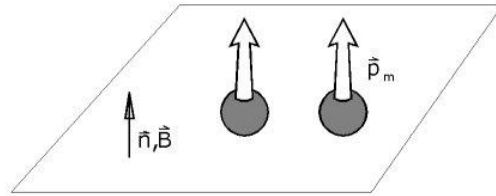
Superparamagnetic colloids in external magnetic field:

$$\mathbf{m}_i = \chi V \left[\mathbf{B}_0 + \sum_j \mathbf{B}_j(\mathbf{r}_i) \right] / \mu_0$$

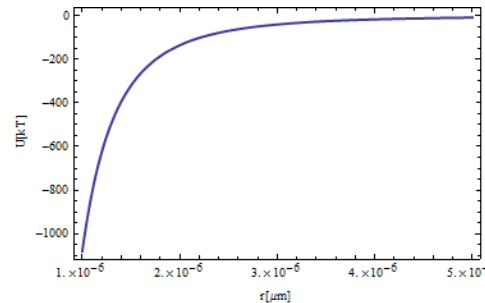
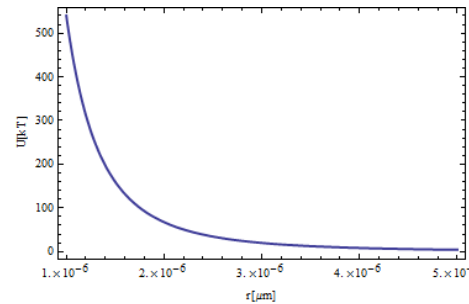
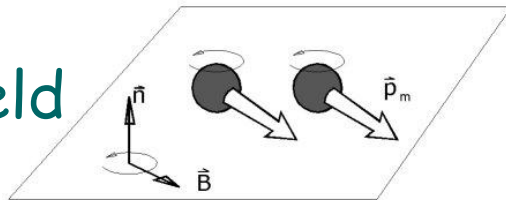
$\sim 1/r^3$ induced interactions



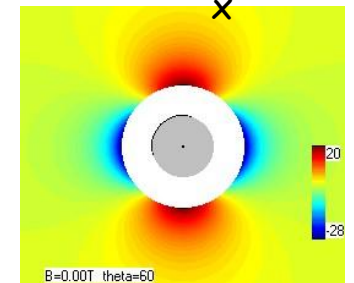
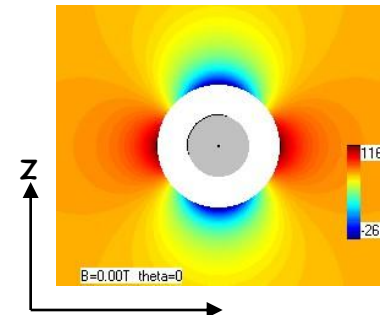
static field



rotating field



movies



Magic Angle Geometry (bulk system)

r^{-3} terms vanish

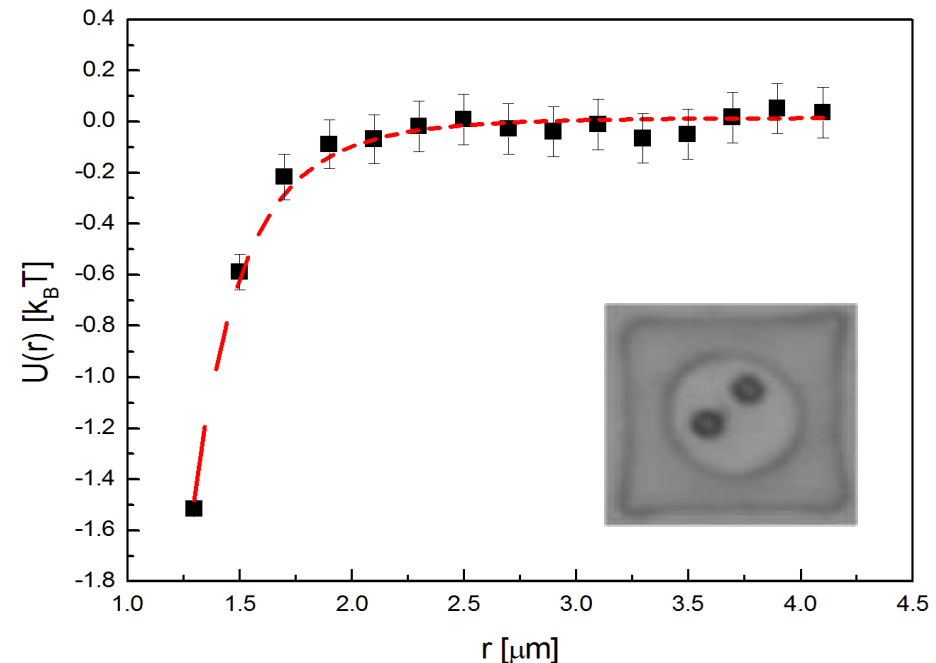
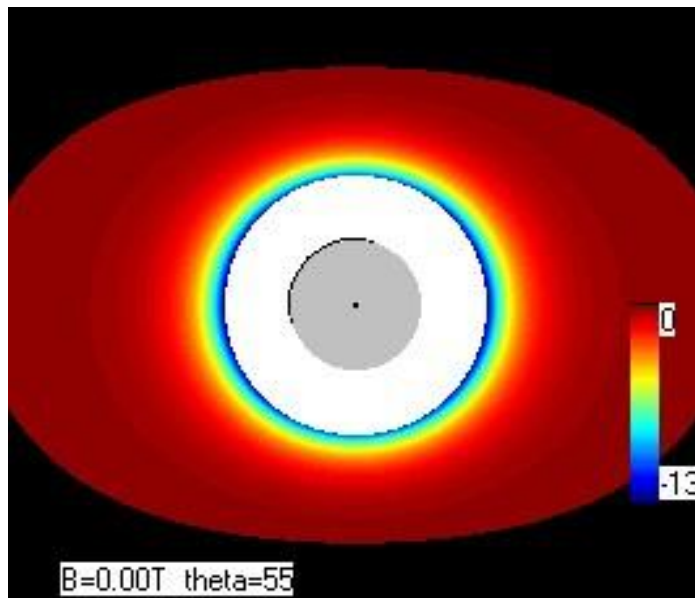
isotropic r^{-6} attraction in 3D!

(SCFI: van der Waals-like)

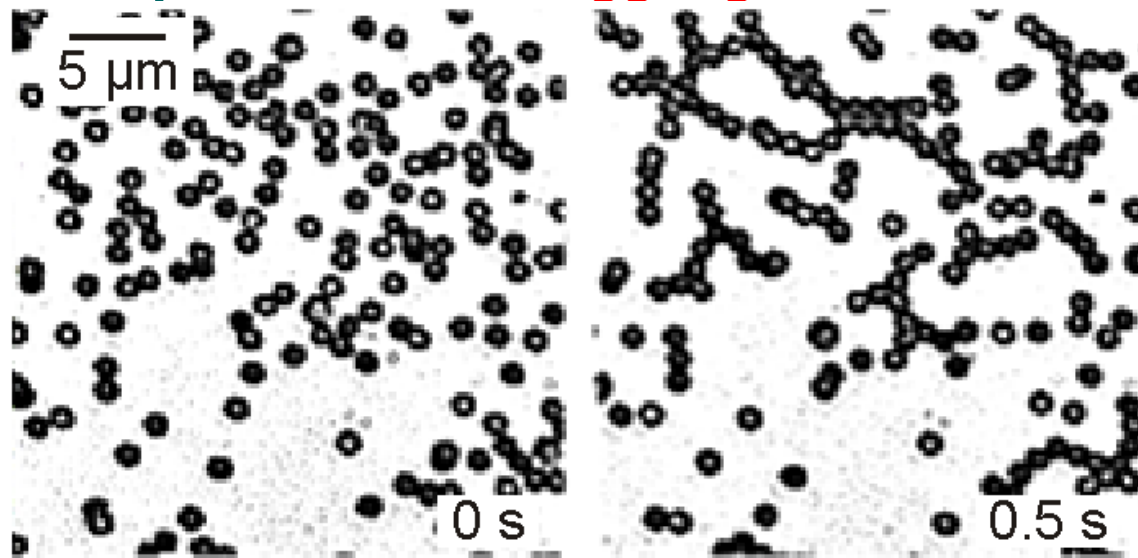
magic angle:

$$\Theta_m = \arccos(1/\sqrt{3}) \approx 54.7^\circ$$

$$U_2(r) = -3\chi^3 V^3 B_0^2 / 8\pi^2 \mu_0 r^6$$



Experiment: aggregation in 3D at magic-angle



dimers and short chains

branching

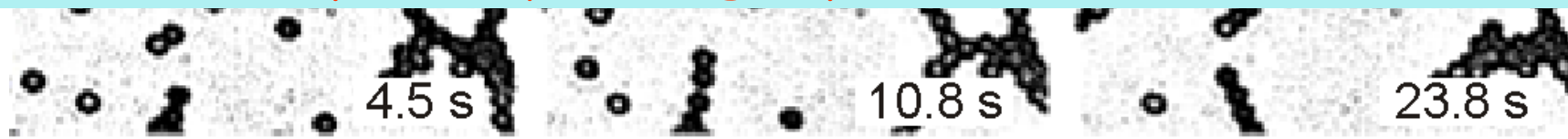
network formation

coarsening and consolidation of membrane patches

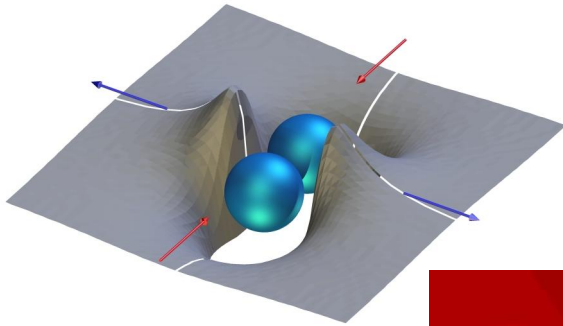
characteristic length-scale $L^* \sim 8$



ordered robust pathway to single-particle thick membranes

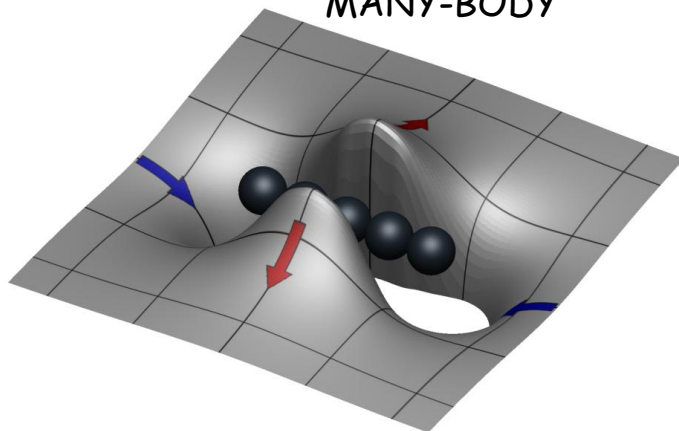
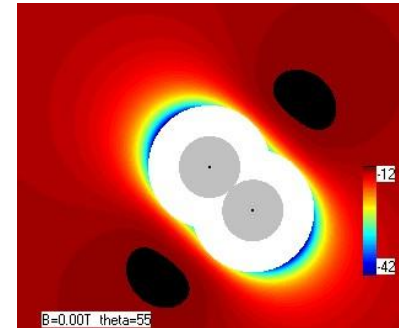
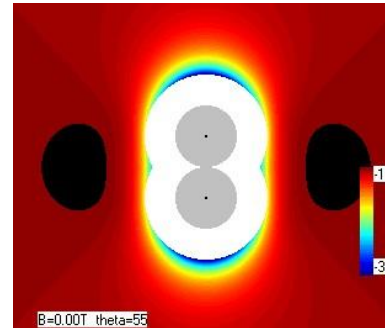
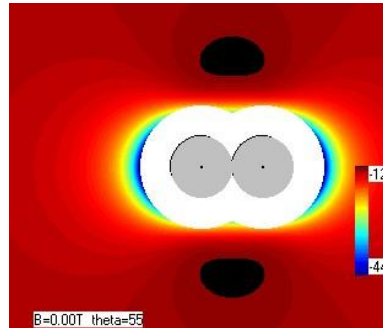


Interaction potential

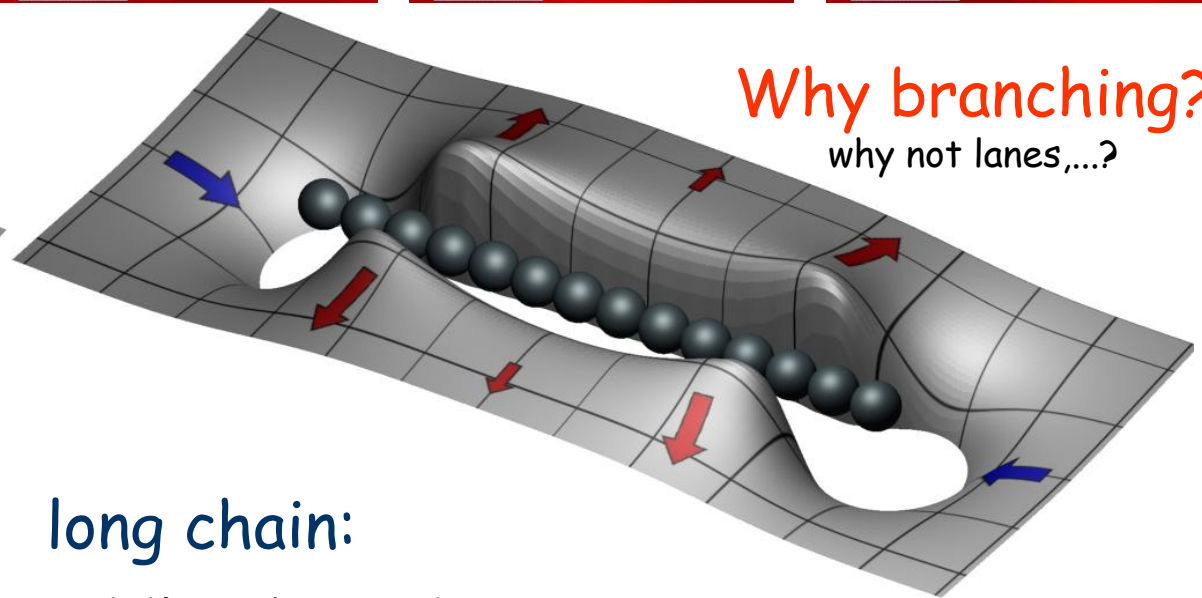


test particle
around dimer

Why chains?
MANY-BODY



short chain:
lateral barrier
 $\sim 1.6 k_B T$



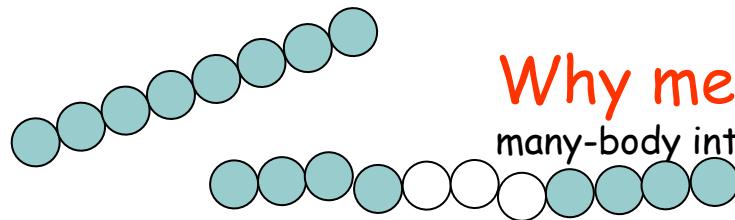
Why branching?
why not lanes, ...?

long chain:
saddle-shaped barrier $\ll 1 k_B T$
 \rightarrow lateral attachment likely for $L \geq 8$ ($=L^*$)

Membranes

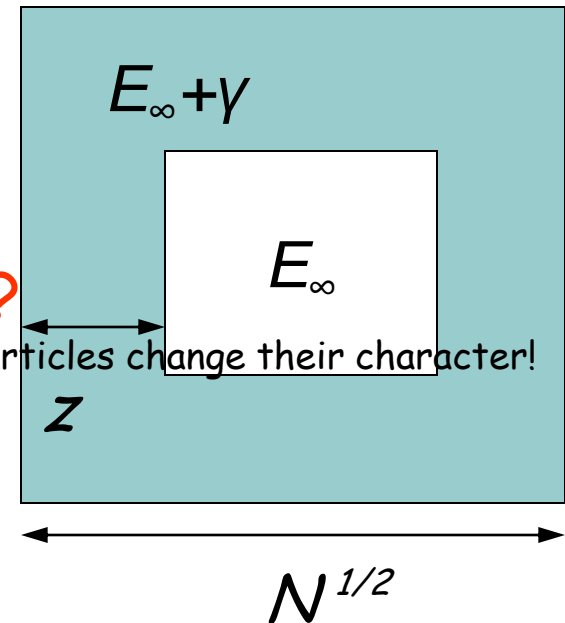
phenomenological model

membranes are stable
chains: core and caps



Why membranes?

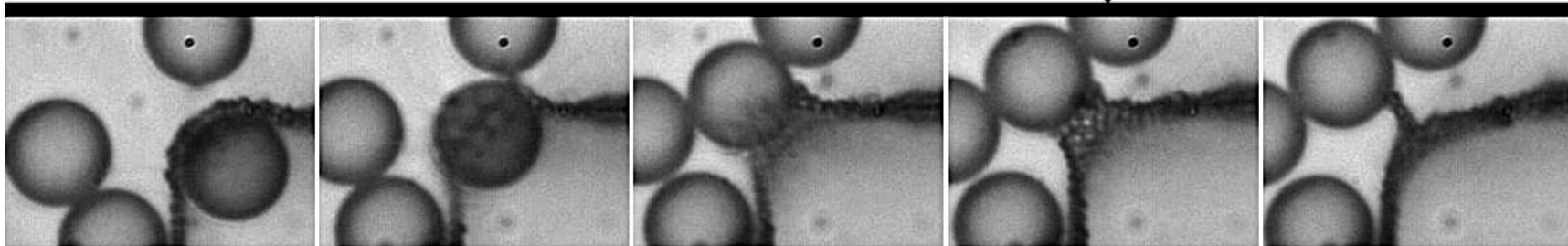
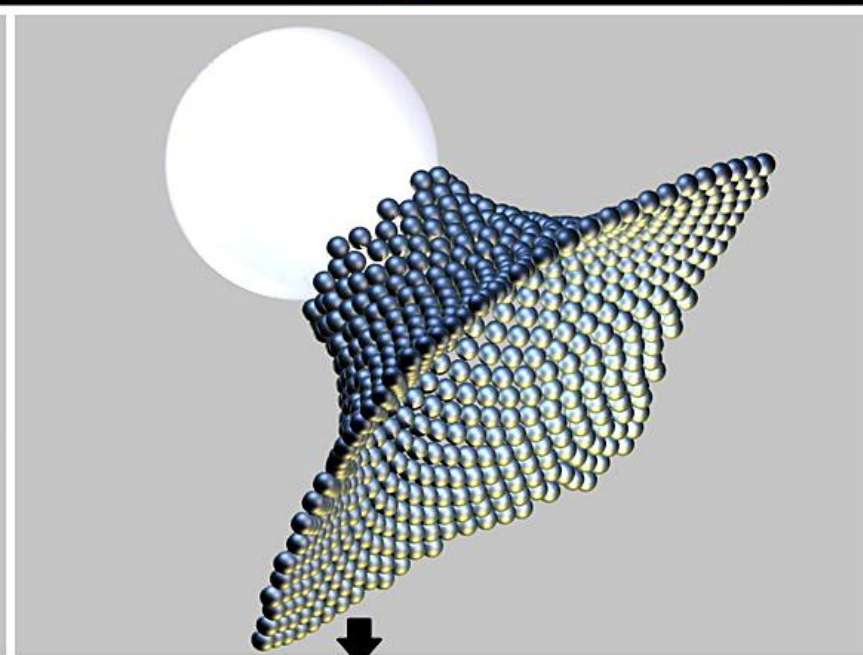
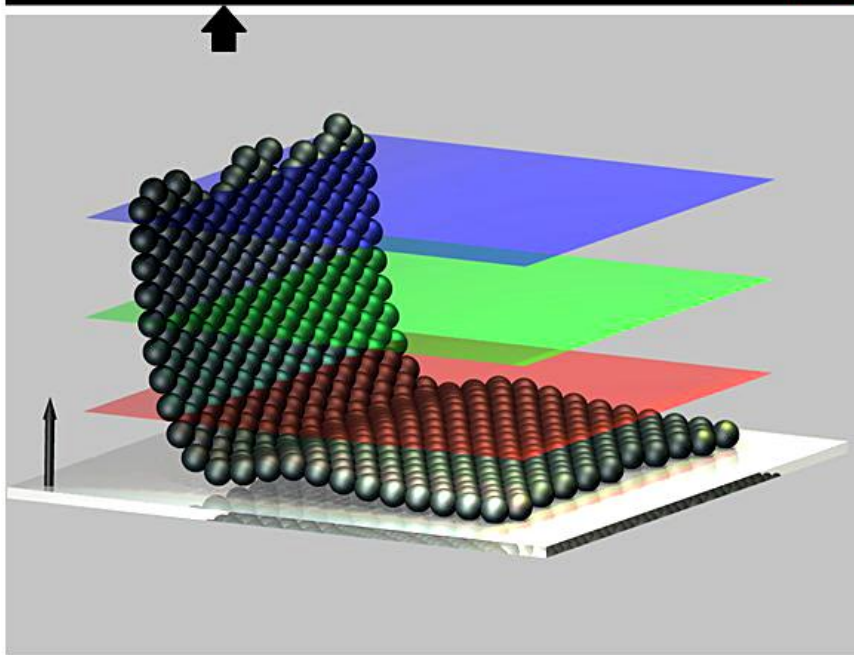
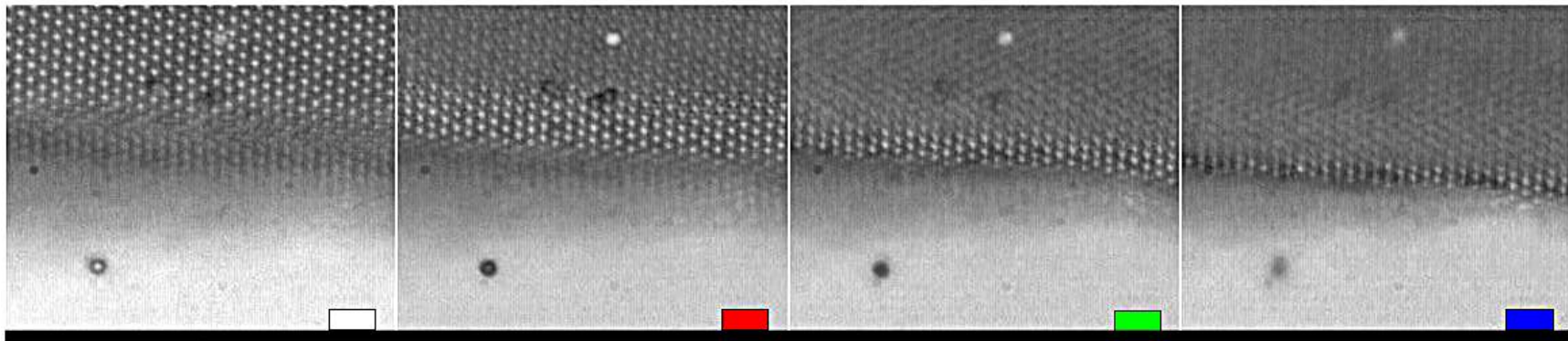
many-body interactions \rightarrow particles change their character!



$L^* = 2$ $z^* = 8$ consistent result

$$E(N) = E_\infty + 4z\gamma N^{-1/2} (1 - zN^{-1/2})$$

$$E_\infty = -119k_B T \quad z^* = 4 \quad \gamma^* = 52k_B T$$

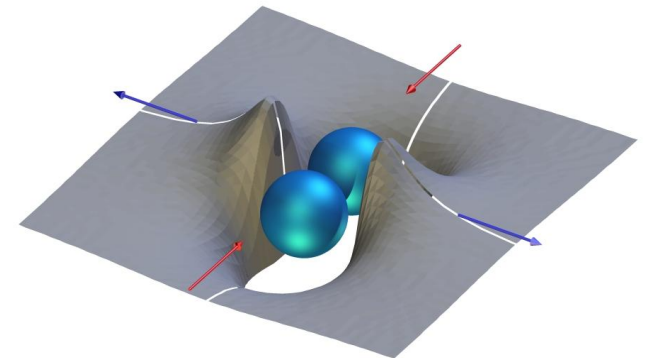
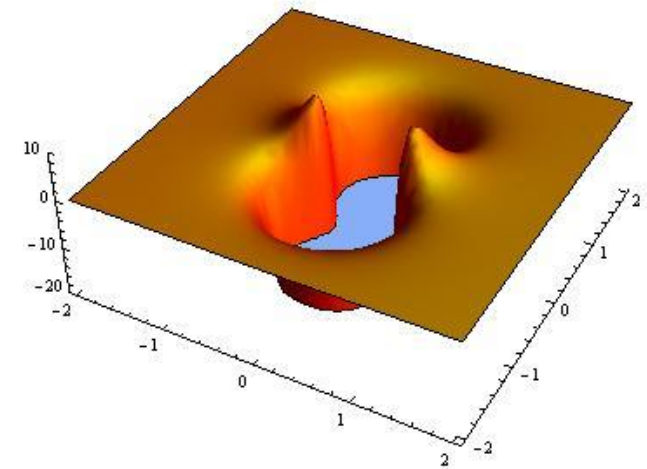


VdW vs SCFI

van der Waals:
decoherent dipole fluctuations
→ weaker many-body effects
→ bulk aggregates, ...

Coherently varying fields:
→ enhanced many-body terms
→ low-dimensional structures

AT 3-body term in VdW



VdW (ICFI) vs SCFI

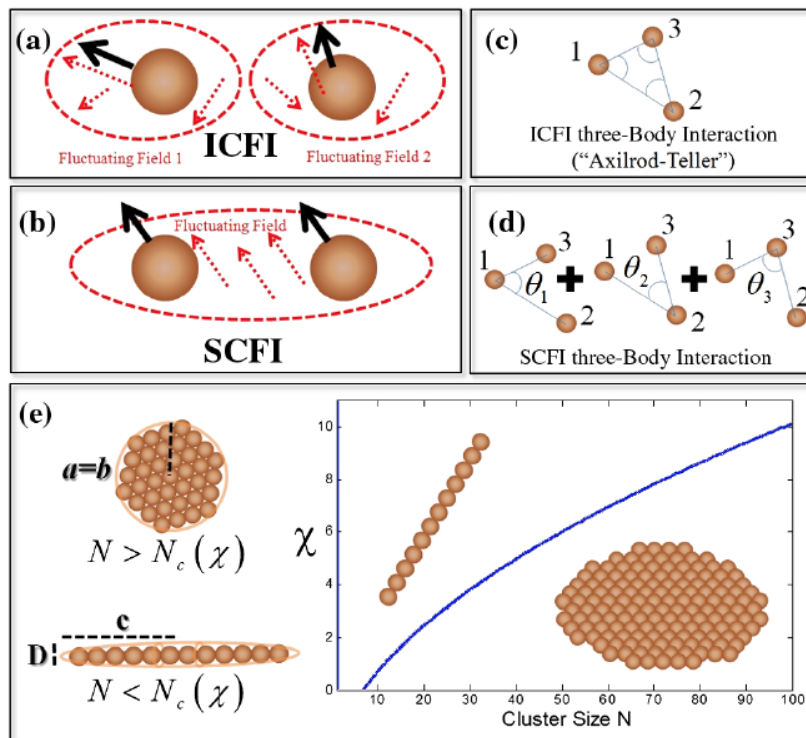
PRL 111, 198301 (2013)

PHYSICAL REVIEW LETTERS

week ending
8 NOVEMBER 2013

Self-Assembly of Colloidal Superstructures in Coherently Fluctuating Fields

Igor M. Kulić^{1,*} and Miodrag L. Kulić^{2,†}



2-body:

$$\sim \chi_b^2 R^{-6}$$

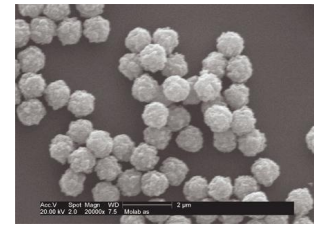
3-body:

$$\sim \chi_b^3 R^{-9}$$

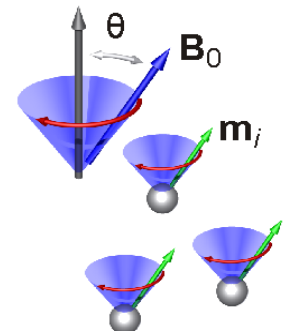
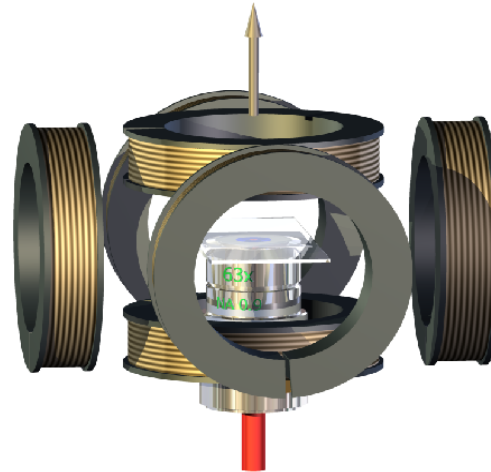
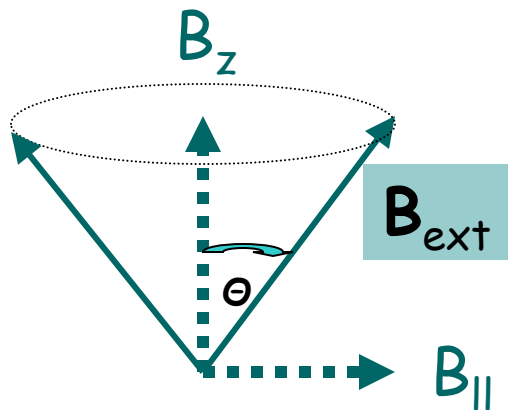
ICFI

$$- \chi_b^3 |\mathbf{R}_{ij}|^{-6}$$

SCFI



Physical rotation of colloids



Flipping the direction \rightarrow suppressing rotation \rightarrow no HD

What happens if we let them rotate?

Hydrodynamics

I. Pagonabarraga: rotators in liquid

Eur. Phys. J. E **26**, 103–113 (2008)

- hexagonal array of rotators is unstable
- inertia (high Re) can stabilize it

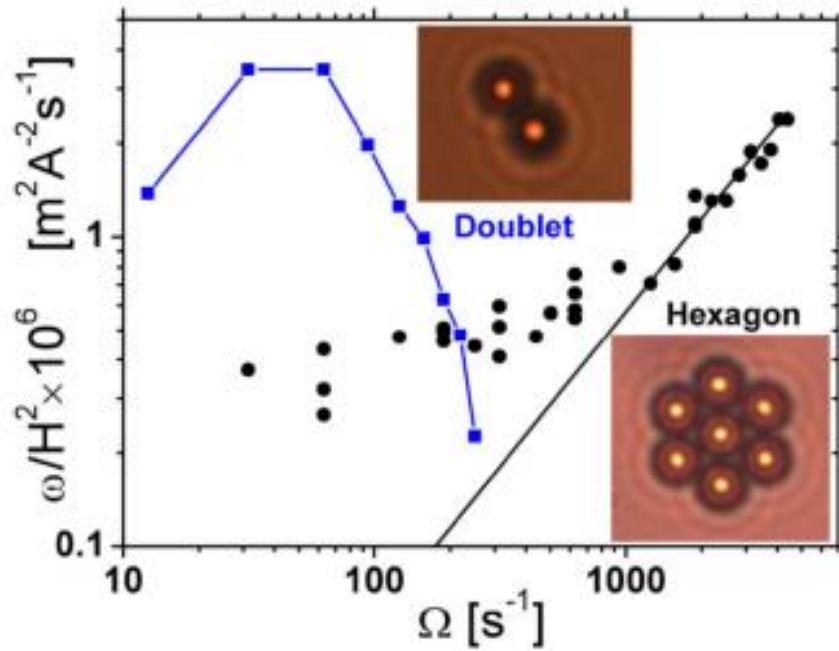
Possible scenario:

- single colloid membrane unstable
(viscous hydrodynamics vs magnetic) \rightarrow vortices (?)
- inertial terms stabilize hexagonal array of vortices (?)

Work in progress...

Rotating clusters (*Fischer et al.*)

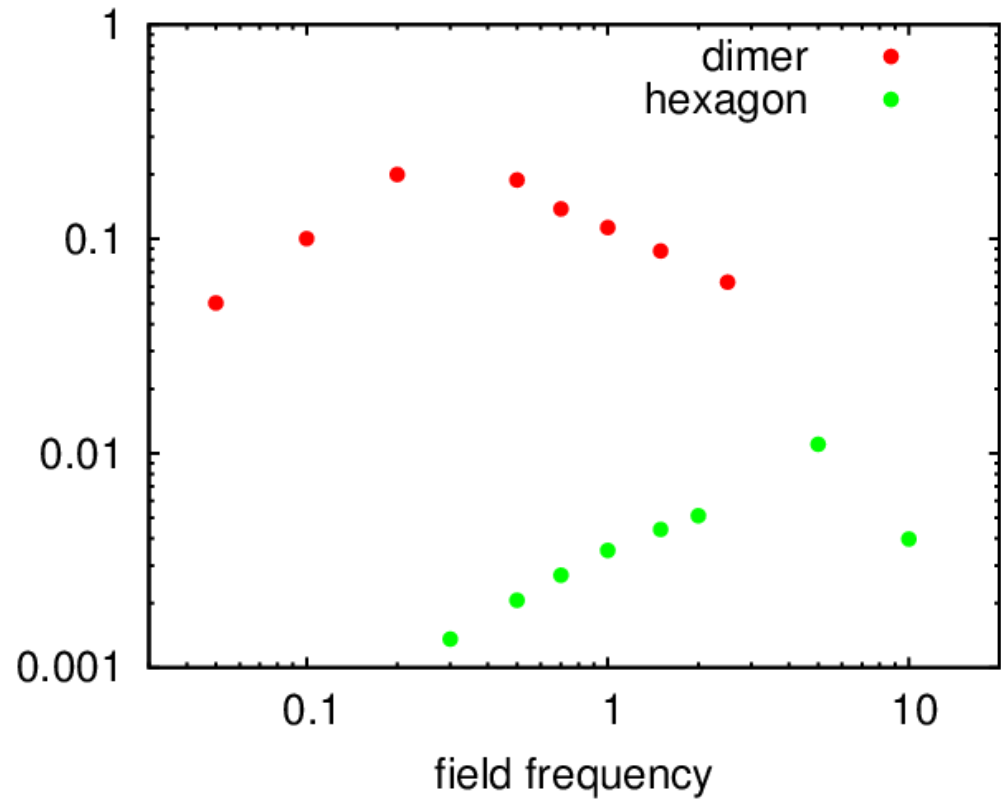
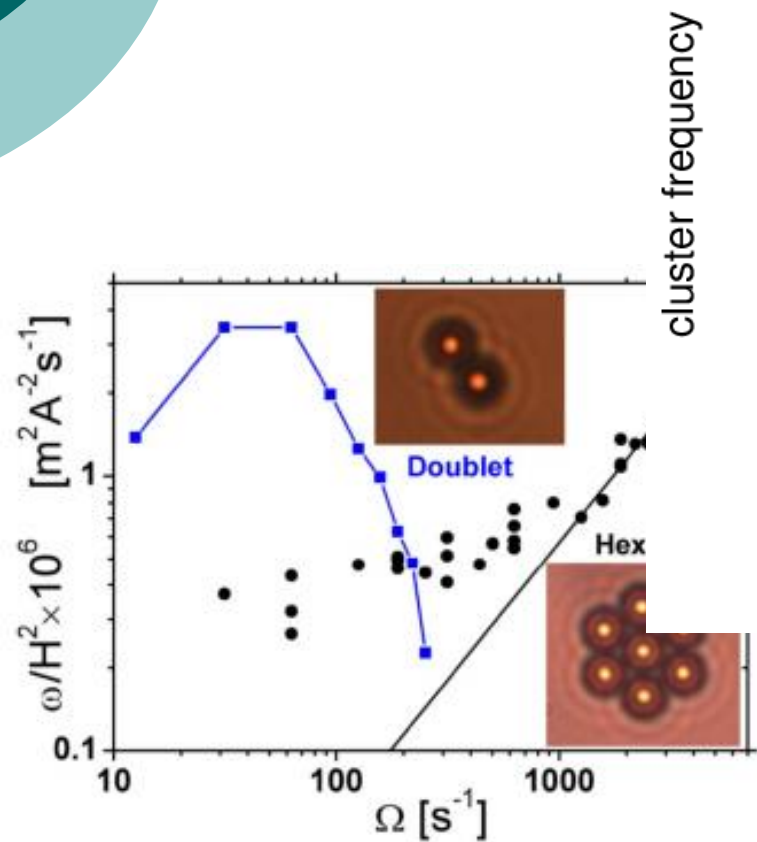
- Chains rotate due to anisotropic susceptibility
- Hexagons rotate due to tidal locking of the shear deformation (*P. Tierno, R. Muruganathan and T.M. Fischer, PRL 2007*)



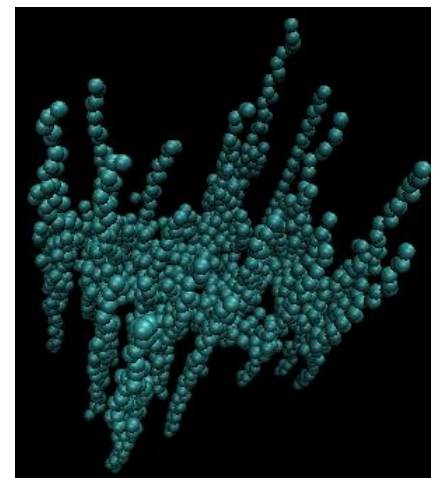
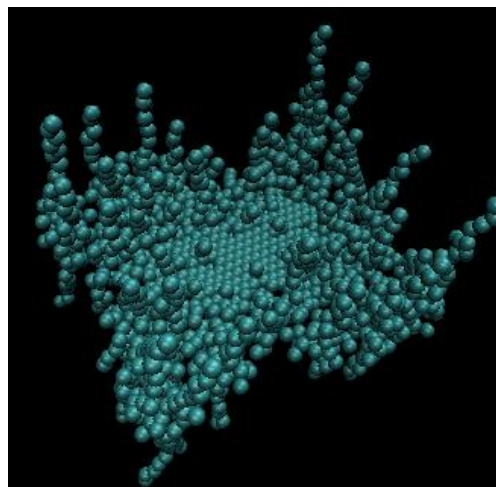
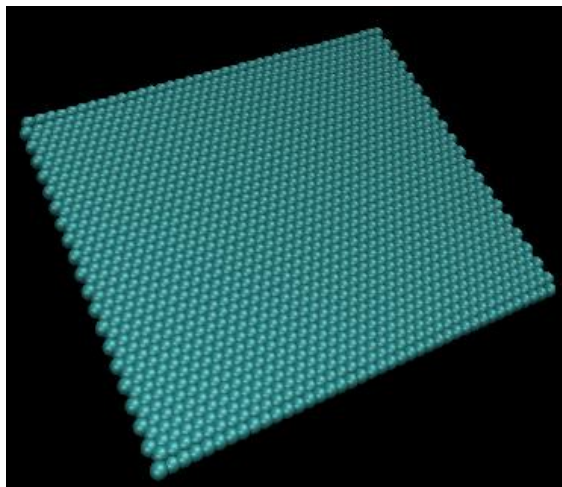
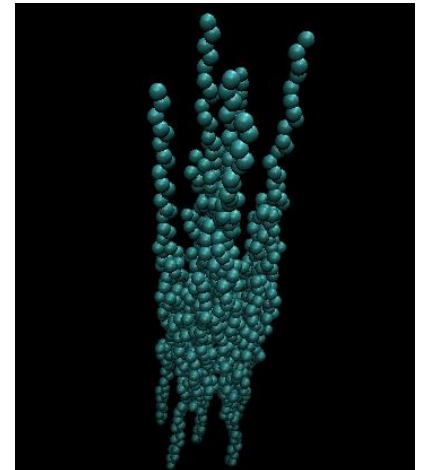
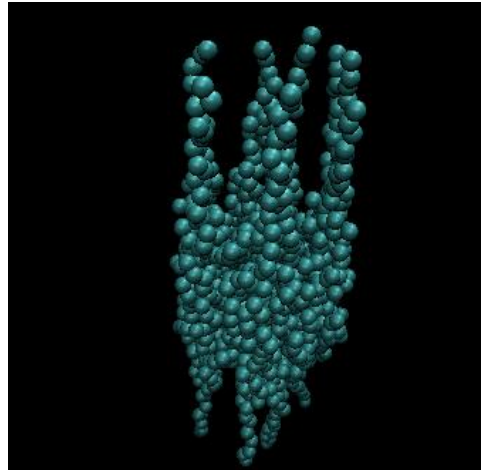
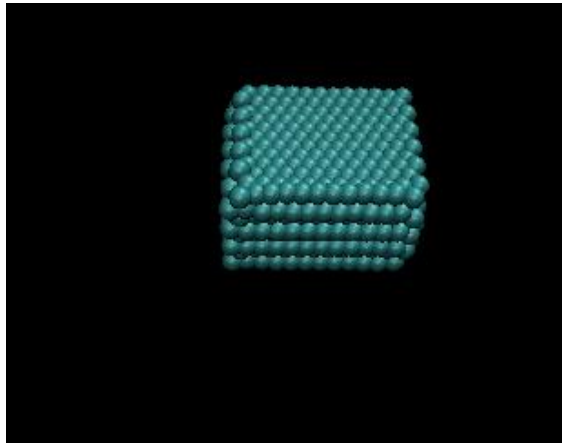
Synchronization-induced structural transition in magnetic Janus colloids:

Jing Yan, Moses Bloom, Sung Chul Bae, Erik Luijten & Steve Granick, *Nature* **491**, 578 (2012)

SIMULATIONS (in progress)



SIMULATIONS (very preliminary)

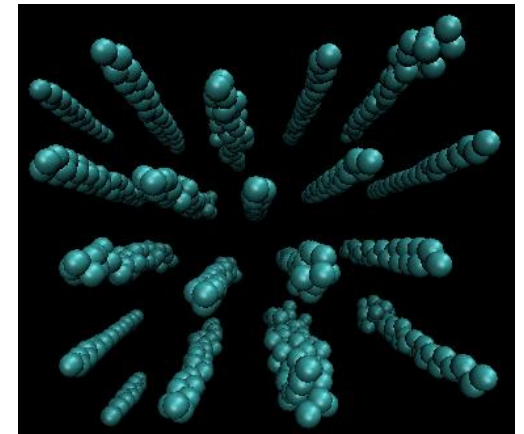
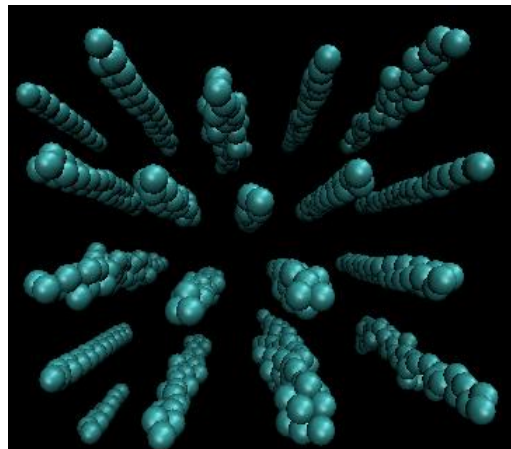
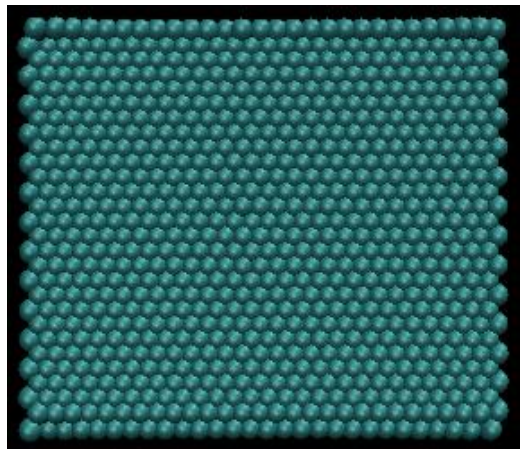
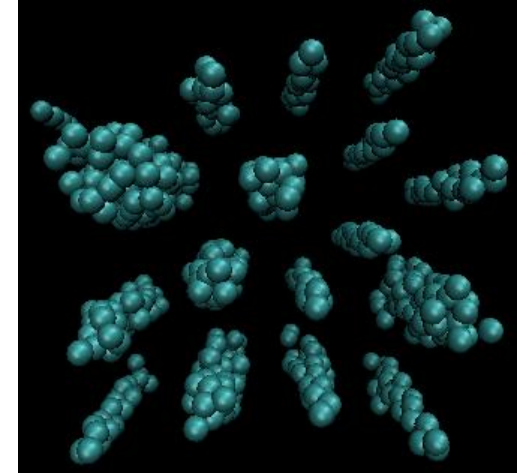
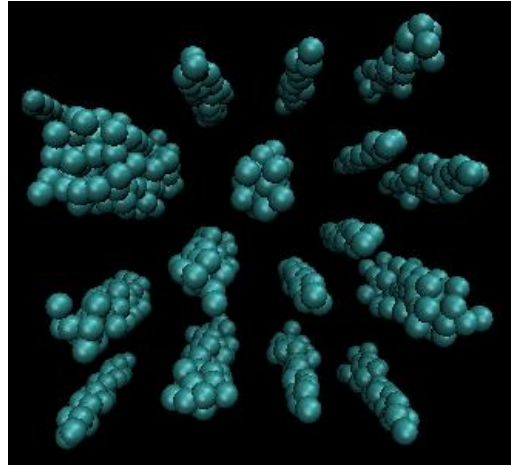
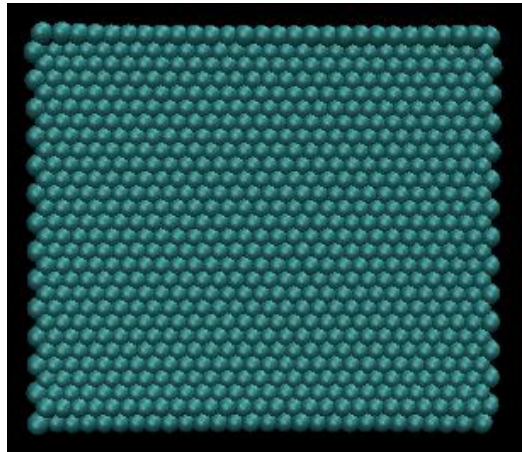


Initial state

10^6 steps

2×10^6 steps

Dependence on initial conditions

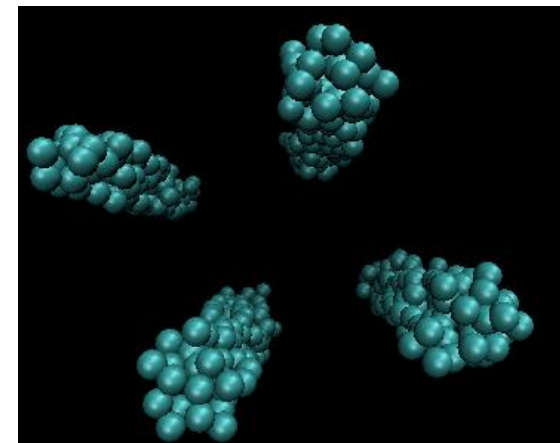
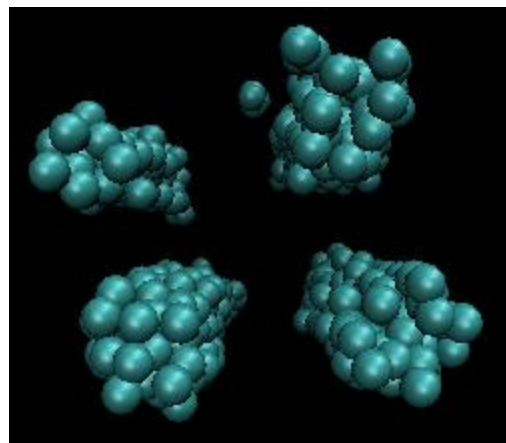
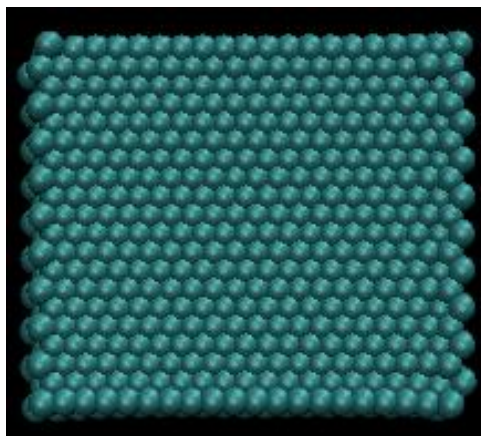
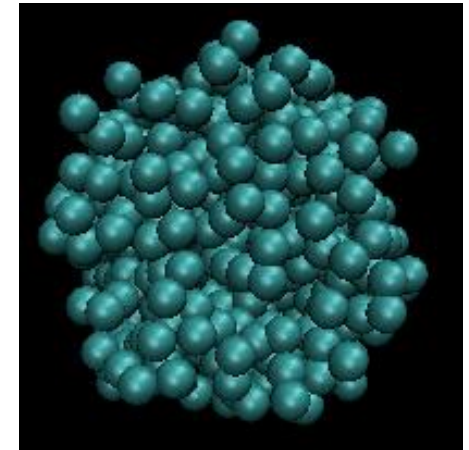
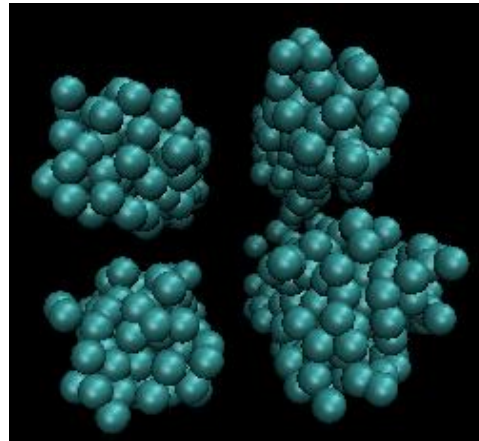
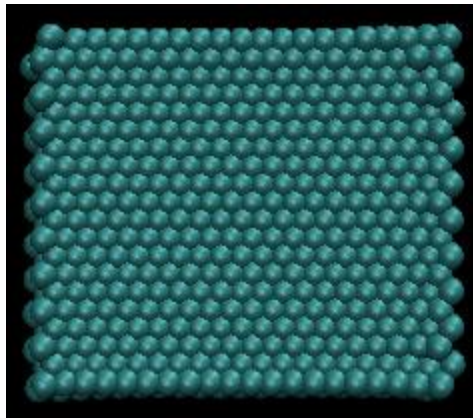


Initial state

10^6 steps

2×10^6 steps

Dependence on initial conditions

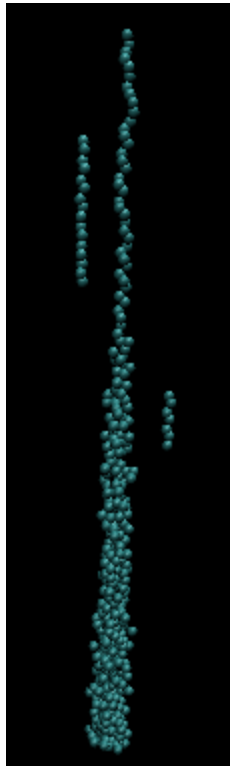


Initial state

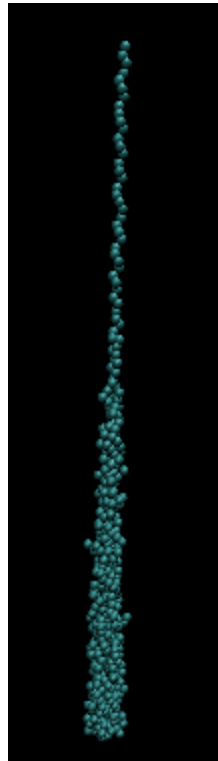
10^6 steps

2×10^6 steps

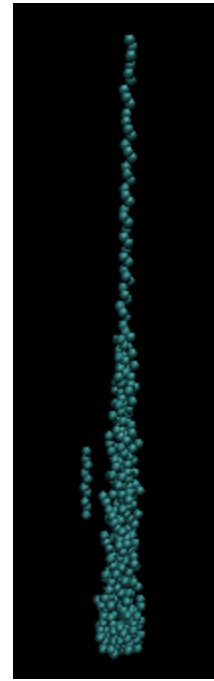
Effect of gravity ...



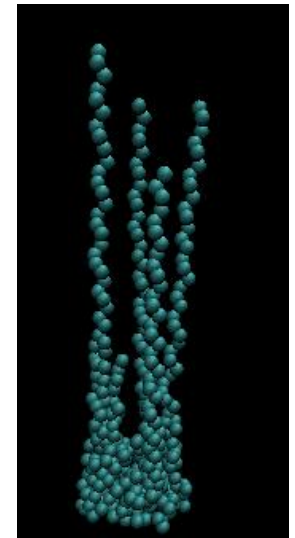
16 mT



10 mT



5 mT



2.5 mT

in progress ...

Conclusions

Rich emergent behaviour

Equilibrium self-assembly:

Low-dimensional structures, closed-shell objects?

Dynamic self-assembly:

we need to understand better what is going on...

Thank you.