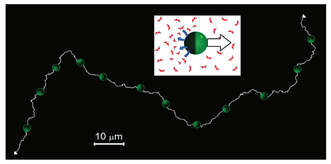
Self-assembly of confined Janus particles

AME Department

Anthony Medrano, Sébastien Michelin and Eva Kanso

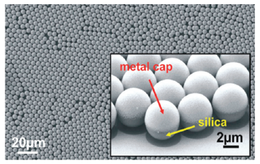
medranoa@usc.edu

Motivation



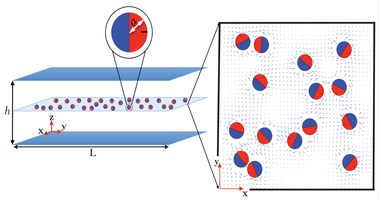
Janus particles are two-sided particles with differing properties, which give rise to its self-propelled motion. These Janus particles are chemical in nature. Each hemisphere produces/consumes ions and is responsible for its autonomous movement.

These nano-/microscale, autonomous particles are relevant in the pursuit of improved drug delivery. By studying their collective behavior, we can gain insight into how they could potentially be employed to effectively deliver drugs to infected sites.



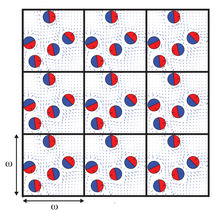
Model

Hele-Shaw Flow



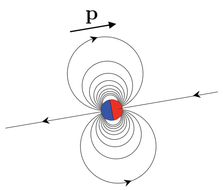
- A doubly-periodic domain is continuous in two directions and eliminates boundary effects

Doubly-Periodic Domain



- The flow field and chemical concentration gradient produced by Janus particles are modeled as source dipoles.
- Conditions for 2D approximation:
  1. a << h (hydrodynamic)
  2. h << L (chemical)

Problem Formulation



$$\dot{\mathbf{x}}_j = \mathbf{p}_j + (\zeta - 3)\mathbf{u}(\mathbf{x}_j) + \mathbf{v}_j$$

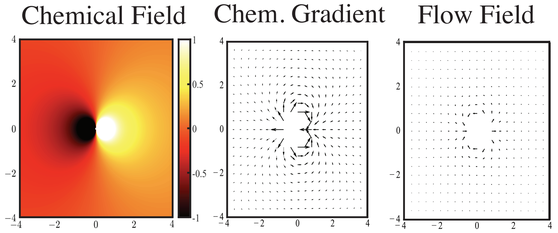
hydrodynamic mobility coefficient

steric repulsion

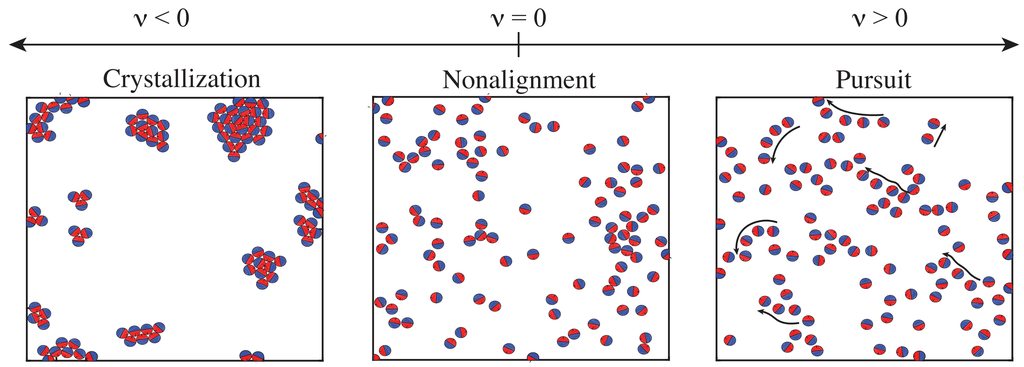
$$\dot{\mathbf{p}}_j = \nu(\mathbf{I} - \mathbf{p}_j \otimes \mathbf{p}_j)\nabla C|_{\mathbf{x}_j}$$

rotational mobility coefficient

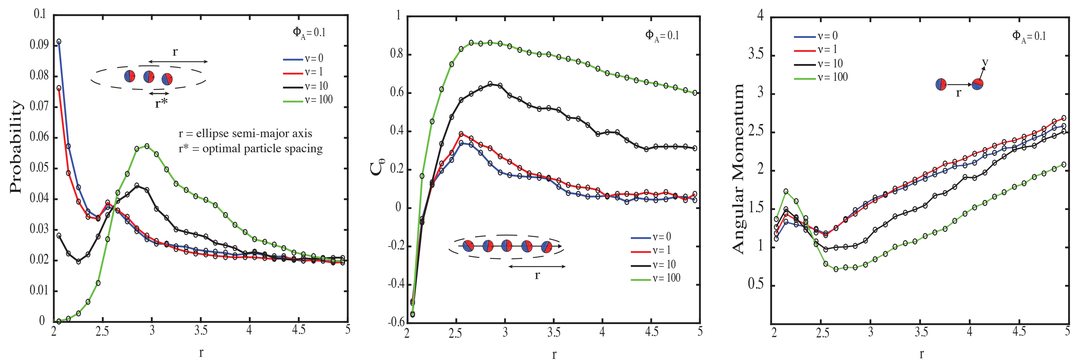
Chemical Field | Chem. Gradient | Flow Field



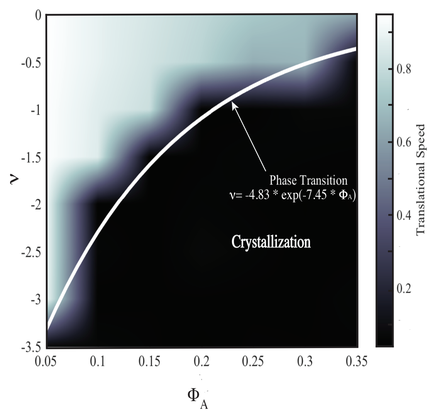
Global Modes

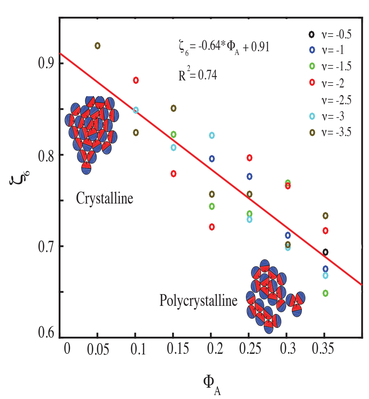


Chains



Crystals

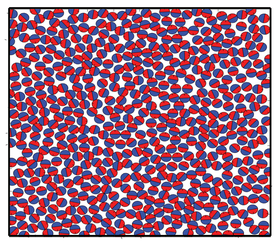




Conclusions

- Three global modes exist: crystallization, nonalignment and pursuit.
- In pursuit mode, chains are formed. Larger rotational mobility coefficients lead to longer, more robust chains. Greater correlation occurs when particles are closer to each other. There is a higher tendency for particles to change orientations near the ends of chains.
- Particles that oppose the local chemical gradient will crystallize. Larger area fractions will lead to the formation of polycrystalline structures, whereas smaller area fractions are more likely to form crystalline structures.
- The transition to the crystallized phase does not always occur when particles oppose the chemical gradient. The threshold is illustrated by an exponential function; above it, particles will not be responsive enough to the gradient to cluster.

Future Work



- Investigate behavior at higher particle densities
- Implement the fast multipole method
- Investigate tracking efficiency

References

1. Ebbens and Howse. *Langmuir*. 2011
2. Baraban, et al. *ACS Nano*. 2012
3. Yeo, et al. *Phys. Rev. Lett*. 2015
4. Tsang, et al. *Phys. Rev. E*. 2014