PhD project: A hybrid particle and field-based soft matter simulation setup

We are looking for a dedicated phd-student to a joint project between Murdoch University in Perth Australia and the Niels Bohr Institute, University of Copenhagen, Denmark. The project requires applying for a Postgraduate Research Scholarship at Murdoch University in collaboration with the PhD supervisors. Applicants with a strong undergraduate track record have a particularly high chance of success. If granted, the scholarship covers tuition fees and tax-free living allowances for a 3-year PhD. You will be jointly enrolled at Murdoch University and University of Copenhagen with the possibility of a double phd-degree from both universities.

Read more about the scholarship here:

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The aim of the project is to develop a hybrid particle and field-based soft matter simulation setup to study self-assembly of complex block copolymer systems. We want to combine the flexibility and dynamics of direct particle based simulation methods with the parameter optimization capabilities of self-consistent field theory. The candidate must possess strong coding skills and a background in physics or nanoscience. Prior knowledge of molecular simulation or field theoretic methods will be an advantage, but not a prerequisite.

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Scientific project description

Self-assembly of AB diblock copolymers is well understood. As a function of composition and chemical incompatibility of chains A and B, they form a range of ordered structures: lamellar, networks, hexagonal cylinders and cubic sphere packings. Recent advances in polymer synthesis now allow almost any imaginable molecular architecture to be made with any number of polymeric species. The first step up from linear systems is an ABC star which has already provided a number of structural surprises: Tiling patterns, quasi-crystallinity, tricontinuous networks and hierarchical chiral assemblies built from achiral building blocks are examples of new features exclusive to star systems. We have for a while explored such complex macromolecules using dissipative particle

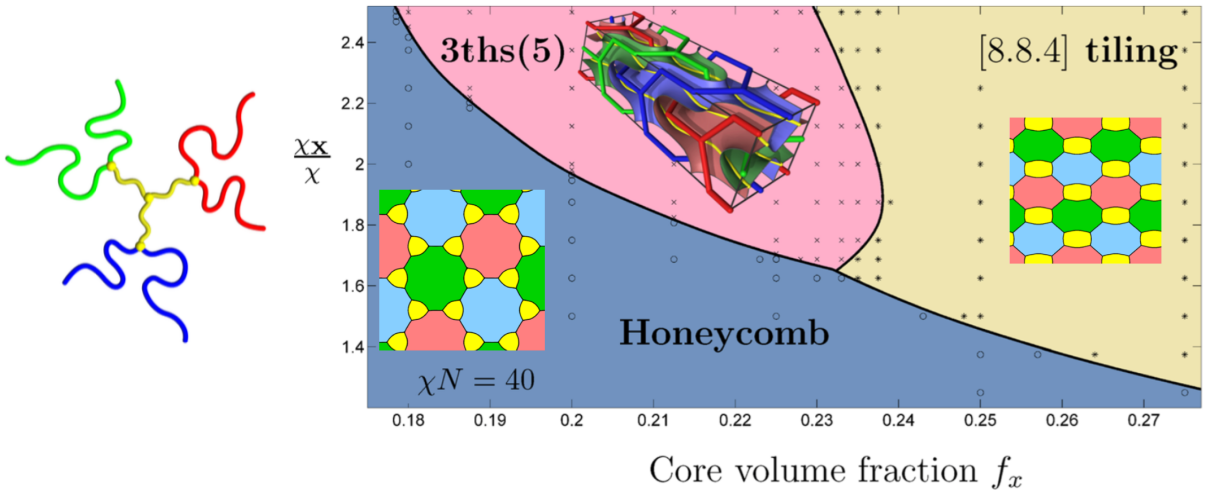

Figure 1: Phase diagram from [9] established by combining **SSCFT** and **DPD**. As a function of the core volume fraction and the interaction strength three structures dominate the phase diagram, one of which is a spectacular tricontinous network structure effectively carving up space into three separated congruent labyrinths, each with a separate chemistry and thus properties.

dynamics (**DPD**) simulations which are a particle based coarse-grained method widely applied to study polymer mesoscale properties [1-9]. However, to reliably predict phase diagrams the dominating computational method is spectral self-consistent field theory (**SSCFT**). The field theory has the advantage that it delivers a free energy so one can build phase diagrams, but has the drawback that it to some extent needs to be told exactly what phases to compare. A common practice in **SSCFT** is to use random initial configurations generated in real- or reciprocal-space. This strategy does reproduce the correct stable phase for simple systems, such as the lamellae or cylinders of diblock copolymers mentioned above, but it also misses many potential candidate structures. For this reason theoretical diblock copolymer phase diagrams have been updated several times during the last 25 years. On the other hand, **DPD** precisely generates new complex structures many of which are often unimaginable [1], but does not easily allow a free energy to be calculated. Thus, the two methods can very briefly be summarized as follows:

- **SSCFT** : estimates free energy, but imposes symmetry group and topology
- **DPD** : relaxation without imposed symmetry/topology constraints, but no estimate of free energy

Here we wish to develop a hybrid setup combining the advantages of these two methods in relation to block copolymer self-assembly. This is possible since the output from **DPD** can be used as input for the **SSCFT** and assigned free energies to build up full phase diagrams. This was successfully part of the strategy in our recent paper [9]. Here we suitably adjusted the molecular architecture and chemistry of ABC stars and showed that this can favour a thermodynamically stable tricontinuous structure based on three intertwined so-called ths-nets [9] (Figure 1). However, the strategy was very brute force with no real computational overlap between the two methods. The **SSCFT** code used in [9] was developed in the group of **GST**. The **DPD** code is using the open source soft matter simulation package Espresso. Thus, the purpose of this phd project is to further develop this combination of methodology to a general powerful hybrid setup capable of reliably exploring the phase space of block copolymers with complex architectures. The main challenges are to establish a robust mapping between the two methods for a given **DPD** coarse-graining, to implement non-cubic box relaxation in the **DPD** setup since one of the parameters which are minimized in the **SSCFT** is

the shape of the unit cell. We also need to properly interface the two methods and provide intelligent output from the setup. The setup should of course be tested and a natural starting point is to reproduce the diblock copolymer phase diagram from a random starting point which has not been achieved before. After that there are numerous questions to address in a very active growing field studying complex self-assembly structures in block copolymer systems. In particular, as the complexity of the structures increases, the experimental determination becomes more and more difficult requiring new advanced analysis tools. On a broader horizon (and obviously a longer timescale), the development of this type of hybrid setup has many potential applications. One example could be to study and understand the formation of the complex and unusual phases found in plant membrane systems, so-called prolamellar bodies, where the length scales are currently a limitation to particle based methods.

[REFERENCES]

[1] **Kirkensgaard J.J.K.**, Evans M, de Campo L and Hyde S.T., **PNAS**, 2014, 111(4), 1271-1276
[2] **Kirkensgaard J.J.K.**, Pedersen M.C., Hyde S.T., **Soft Matter**, 2014, 10, 7182-7194 (2014 Hot Paper)
[3] **Kirkensgaard J.J.K.**, **Physical Review E**, 2012, 85, 031802
[4] **Kirkensgaard J.J.K.**, **Interface Focus**, 2012, 2 (5), 602-607
[5] **Kirkensgaard, J.J.K.** and Hyde, S., **PCCP**, 2009, 11, 2016-2022
[6] **Kirkensgaard J.J.K.**, **Soft Matter**, 2010, 6, 6102-6108
[7] **Kirkensgaard, J.J.K.**, **Soft Matter**, 2011, 7, 10756
[8] **Kirkensgaard J.J.K.**, Fragouli P, Hadjichristidis N and Mortensen K, **Macromolecules**, 2011, 44 (3), 575-582
[9] Fischer MG, de Campo L, **Kirkensgaard J.J.K.**, Hyde ST and **Schröder-Turk GE**, **Macromolecules**, 2014, 47, 7424-7430
[10] Fischer MG, Hyde ST, **Schröder-Turk GE**, Soft Matter, 2015 Feb 14;11(6):1226-7