Dynamics of pattern-forming and self-assembing soft nanostructured materials

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Scientific Thrust Area and Relevant Molecular Foundry Proposals

The Theory Facility at the Molecular Foundry seeks to understand the principles that underpin the self-assembly and organization of 'soft' materials comprised of nanoscale components bound together by forces comparable to thermal forces. Guided by the simple ideas and unifying principles of statistical mechanics, we we work in collaboration with experimentalists to understand the dynamics through which nanoscale components, both biological and inorganic, associate. Here we present an overview of work from three current collaborations: the *in vitro* crystallization of of bacterial S-layer proteins (with the DeYoreo and Bertozzi groups, Molecular Foundry); the self-assembly of functionalized peanut-shaped colloids (with the Bon Group, Warwick University, User project *Assembly of Anisotropic Particles and their Interaction with Soft Interfaces*); and pattern-forming dynamics of nanostructured actin networks *in vivo* (with T. Bretschneider and N.J. Burroughs, Warwick University).

Research Achievements, resulting publications, and future work

- *S-layer protein crystallization.* Demonstrated that a minimal model of associating monomers with competing nonspecific and specific ('lock-and-key') interactions can mimic experimentally observed crystallization dynamics. We are exploring this model to identify the design principles by which protein-protein interactions select their dynamic assembly pathway [Fig. 1].

- *Peanut-shaped colloid assembly* (User project with S.A.F. Bon): Used molecular simulation to identify morphologies of colloidal assemblies accessible to functionalized peanut-shaped colloids as a function of peanut shape. We are currently comparing theory and experiment, and plan to use the theoretical program to help design novel colloidal assemblies. Manuscript in preparation.

- Actin network pattern-forming dynamics: Demonstrated that dynamics of nanostructured actin cytoskeleton in single-celled *Dictyostelium* can be reproduced by a continuum reaction-diffusion dynamics. S. Whitelam, T. Bretschneider and N.J. Burroughs, *Phys. Rev. Lett.*, in press.

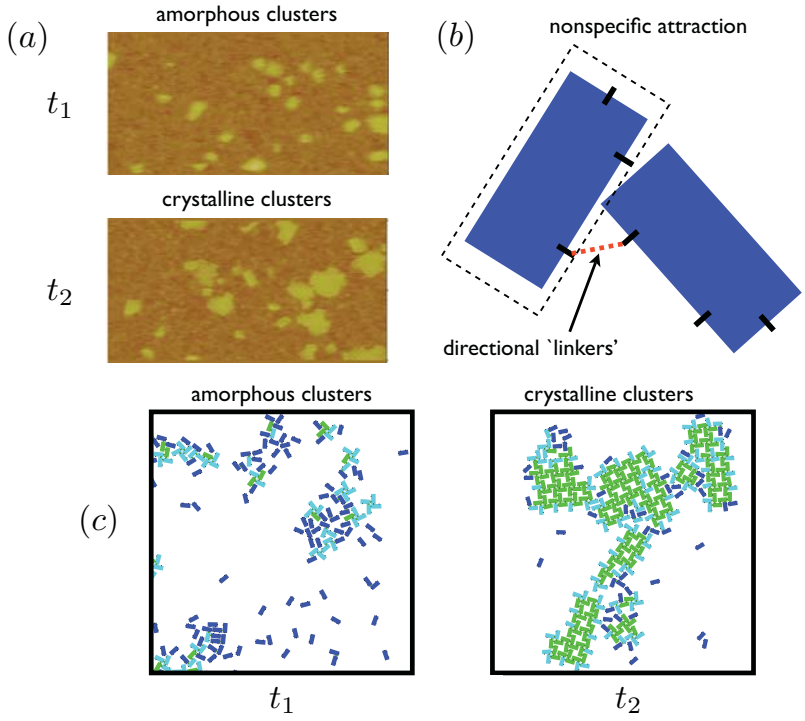

FIG. 1: (a) Bacterial S-layer proteins form, on lipid bilayers, amorphous clusters that spontaneously order and become crystalline on a timescale of minutes [DeYoreo and Bertozzi groups, Molecular Foundry]. (b) A statistical mechanical model of hard rectangles ('monomers') equipped with both nonspecific attractions and directional 'linkers' can (c) recapitulate this complex dynamics. Such models offer insight into the 'design principles' underlying biological assemblies, and allow systematic exploration of the competing roles of phase separation and phase ordering that operate here and in myriad other systems.