# Berkeley Lab postdoctoral position: Theory and simulation of *in vitro* bacterial S-layer protein crystallization

**Summary.** Work with theorists and experimentalists at the Molecular Foundry at Lawrence Berkeley National Laboratory to develop computational statistical mechanical models of the self-organization of bacterial S-layer proteins. The aim of this research is to clarify the thermodynamic and kinetic factors that control the multi-stage crystallization of S-layer proteins observed in Foundry experiments, and to advance general understanding of the self-organization of anisotropically-interacting nanoscale components.

This two-year postdoctoral appointment complements an experimental postdoctoral position that will focus on using fluorescence data to clarify S-layer protein mobility and conformational flexibility.

**Background.** S ('surface')-layer proteins form crystalline lattices on the outsides of many bacteria and archaea. While the lattice structures of many S-layers are known, their dynamics of formation is poorly understood. In an effort to provide such understanding, the DeYoreo and Bertozzi groups at the Molecular Foundry have used atomic force microscopy to image in real time the deposition of a certain S-layer protein on a supported lipid bilayer. The dynamics of crystallization is complex: proteins first aggregate into amorphous clusters, which subsequently acquire square crystalline order. We have developed a simple statistical mechanical model that qualitatively recapitulates this behavior (pictured): this position will focus on the in-depth analysis and further development of this model to permit quantitative comparison with existing and planned in-house experiments.

*The Molecular Foundry at Lawrence Berkeley National Laboratory is a user facility for the design, synthesis and characterization of materials with nanometer dimensions. One of five such Nanoscale Science Research Centers recently established by the U.S. Department of Energy, its charter defines two primary missions: a) conduct outstanding research across the breadth of nanoscience; and b) collaborate with scientists from around the world who visit to use its state-of-the-art instruments, techniques and expertise to further their own nanoscience research efforts* (`http://foundry.lbl.gov`).

**Qualifications required.** Ph.D. in theoretical condensed matter physics, chemistry, materials science, or a related discipline whose focus is the study of phase transformations in dynamically complex materials such as glasses, gels, colloids, polymers etc. Expertise in the construction, analysis and simulation of coarse-grained models of such materials is essential. Experience with advanced computational methods for the determination of thermodynamic phase diagrams of isotropic and 'patchy' particles is highly desirable.

**To apply:** Please email CV and cover letter to Dr. Steve Whitelam (`swhitelam@lbl.gov`), Theory of Nanostructured Materials Facility, The Molecular Foundry, Lawrence Berkeley National Lab.

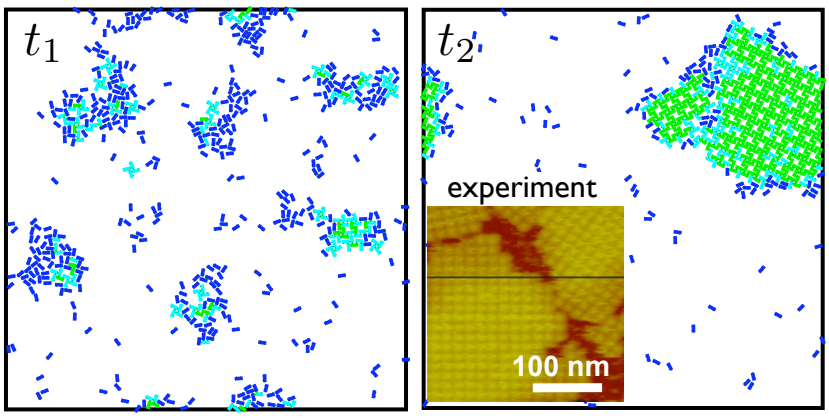


FIG. 1: Statistical mechanical model of S-layer assembly: anisotropically-interacting nanoparticles exhibit 'two-step' ordering into square crystal lattice. Inset: AFM image of *in vitro* assembled S-layer.