LBNL postdoctoral position in theory and simulation

Protein-mimetic materials for molecular recognition and catalysis: Design and simulation of coarse-grained molecular models of peptoid polymers

Summary. Work with theorists and experimentalists at the Molecular Foundry at Lawrence Berkeley National Laboratory (LBNL) to develop a coarse-grained molecular simulation model of peptoid nanostructure self-assembly.

Background. The postdoctoral fellow will join a multidisciplinary team whose goal is to combine synthesis, characterization and computer simulation in order to extend the rules that govern protein structure and folding to the world of non-natural polymers. Peptoids are polymers that combine the specificity of proteins and the stability of polymers. Like proteins, peptoids are composed of a precise sequence of chemically distinct monomers, can fold and self-assemble into defined architectures, and can have potent biological activities. However, they can also incorporate a much wider range of chemical functionalities, are considerably more stable, and are easy to synthesize. The project aim is to design a new class of peptoid-based molecular sensors that combine the specificity of proteins and the robustness of polymers.

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 Nanoscale Science Research Centers 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, structural biology, or a related discipline whose focus is the study of phase transformations in dynamically complex materials such as glasses, gels, colloids, (bio)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. Familiarity with atomistic simulation is desirable.

To apply: Please send CV, cover letter, and three references to Dr. Steve Whitelam (`swhitelam@lbl.gov`), and see posting at `jobs.lbl.gov` .