MAR17-2016-001464

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

2-d and 1-d Nanomaterials Construction through Peptide Computational Design and Solution Assembly[1]

DARRIN POCHAN, University of Delaware

Self-assembly of molecules is an attractive materials construction strategy due to its simplicity in application. By considering peptidic molecules in the bottom-up materials self-assembly design process, one can take advantage of inherently biomolecular attributes; intramolecular folding events, secondary structure, and electrostatic/H-bonding/hydrophobic interactions to define hierarchical material structure and consequent properties. Importantly, while biomimicry has been a successful strategy for the design of new peptide molecules for intermolecular assembly, computational tools have been developed to de novo design peptide molecules required for construction of pre-determined, desired nanostructures and materials. A new system comprised of coiled coil bundle motifs theoretically designed to assemble into designed, one and two-dimensional nanostructures will be introduced. The strategy provides the opportunity for arbitrary nanostructure formation, i.e. structures not observed in nature, with peptide molecules. Importantly, the desired nanostructure was chosen first while the peptides needed for coiled coil formation and subsequent nanomaterial formation were determined computationally. Different interbundle, two-dimensional nanostructures are stabilized by differences in amino acid composition exposed on the exterior of the coiled coil bundles. Computation was able to determine molecules required for different interbundle symmetries within two-dimensional sheets stabilized by subtle differences in amino acid composition of the inherent peptides. Finally, polymers were also created through covalent interactions between bundles that allowed formation of architectures spanning flexible network forming chains to ultra-stiff polymers, all with the same building block peptides. The success of the computational design strategy is manifested in the nanomaterial results as characterized by electron microscopy, scattering methods, and biophysical techniques.

[1]Support from NSF DMREF program under awards DMR-1234161 and DMR-1235084