

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Computational Analysis of β -Peptide Self-Assembly¹ MICHAEL MCGOVERN, University of Wisconsin-Madison — β -peptides are a class of synthetic oligomers that are capable of folding in precise patterns. The wide variety of side chains that are available for insertion into β -peptide sequences along with the stability of these folded secondary structures allow precise control over the nanoscale presentation of various chemical functional groups in three dimensional space. Some β -peptides have been shown to spontaneously fold into complex supramolecular structures, and others have been shown to be effective antimicrobial agents that are believed to act by aggregating in certain types of cell membranes. However, more work is needed to understand what drives this assembly in order to design β -peptides that assemble in particular ways. Using molecular simulations, the process of β -peptide aggregation is examined in a variety of environments that allow for direct comparison to experiment. Using new simulation techniques, the structure of the aggregates formed by several β -peptides are predicted in both bulk solutions, and at interfaces. Free energy surfaces are generated using multiple geometric parameters to directly compare the favorability of different modes of aggregation. By analyzing these results, we gain an understanding of the factors that drive self-assembly and aggregation.

¹Nanoscale Science and Engineering Center on Templated Synthesis and Assembly at the Nanoscale. We gratefully acknowledge funding from the National Science Foundation, DMR-0832760

Michael McGovern
University of Wisconsin-Madison

Date submitted: 19 Nov 2010

Electronic form version 1.4