Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Sequence-directed organization in self-assembled monolayers of beta-peptides on solid surfaces: A Monte Carlo simulation study[1] JAGANNATH MONDAL, University of Wisconsin Madison, BONG JUNE SUNG, Sogang University, ARUN YETHIRAJ, University of Wisconsin Madison — The sequence-directed organization of self-assembled monolayers (SAM) of amphiphilic β-peptides adsorbed on gold surfaces is studied using Monte Carlo simulations. A phenomenological model is considered where each (helical) molecule is represented by a rigid nano-rod with the side groups at appropriate locations. This model effectively distinguishes between two, namely globally amphiphilic (GA) and non-globally amphiphilic(non-GA), sequence-isomers of an amphiphilic β peptide Y-(ACHC-ACHC-K)$_3$. The simulations show that the GA isomers have a high degree of orientational order that is not exhibited by the non-GA isomers, consistent with experiment. The simulations quantify a subtle balance between electrostatic, hydrophilic, and hydrophobic interactions on the self-assembly of β-peptides on surfaces.

[1]NSF grant DMR-0425880

Jagannath Mondal
University of Wisconsin Madison

Date submitted: 18 Nov 2008 Electronic form version 1.4