Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Molecular Dynamics Simulations of Hydrophobic Residues[1]
DIEGO CABALLERO, ALICE ZHOU, LYNNE REGAN, COREY O'HERN, Yale University — Molecular recognition and protein-protein interactions are involved in important biological processes. However, despite recent improvements in computational methods for protein design, we still lack a predictive understanding of protein structure and interactions. To begin to address these shortcomings, we performed molecular dynamics simulations of hydrophobic residues modeled as hard spheres with stereo-chemical constraints initially at high temperature, and then quenched to low temperature to obtain local energy minima. We find that there is a range of quench rates over which the probabilities of side-chain dihedral angles for hydrophobic residues match the probabilities obtained for known protein structures. In addition, we predict the side-chain dihedral angle propensities in the core region of the proteins T4, ROP, and several mutants. These studies serve as a first step in developing the ability to quantitatively rank the energies of designed protein constructs. The success of these studies suggests that only hard-sphere dynamics with geometrical constraints are needed for accurate protein structure prediction in hydrophobic cavities and binding interfaces.

[1]NSF Grant PHY-1019147

Diego Caballero
Yale University

Date submitted: 09 Nov 2012 Electronic form version 1.4