Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Side-chain mobility in the folded state of Myoglobin HEIKO LAMMERT, JOSE ONUCHIC, Rice Univ — We study the accessibility of alternative side-chain rotamer configurations in the native state of Myoglobin, using an all-atom structure-based model. From long, unbiased simulation trajectories we determine occupancies of rotameric states and also estimate configurational and vibrational entropies. Direct sampling of the full native-state dynamics, enabled by the simple model, reveals facilitation of side-chain motions by backbone dynamics. Correlations between different dihedral angles are quantified and prove to be weak. We confirm global trends in the mobilities of side-chains, following burial and also the chemical character of residues. Surface residues loose little configurational entropy upon folding; side-chains contribute significantly to the entropy of the folded state. Mobilities of buried side-chains vary strongly with temperature. At ambient temperature, individual side-chains in the core of the protein gain substantial access to alternative rotamers, with occupancies that are likely observable experimentally. Finally, the dynamics of buried side-chains may be linked to the internal pockets, available to ligand gas molecules in Myoglobin.

Heiko Lammert
Rice Univ

Date submitted: 11 Nov 2016 Electronic form version 1.4