Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Dynamics of Protein Carbonmonoxyhemoglobin on Multiple Length Scales JYOTSANA LAL, ROBERT FISCHETTI, LEE MAKOWSKI, Argonne National Laboratory, Argonne IL-60439, USA., PETER FOUQUET, MARCO MACCARINI, Institut Laue-Langevin, 38042 Grenoble- Cedex 9, France, NANCY HO, CHIEN HO, Carnegie Mellon Univ., Pittsburgh, PA-15213, USA. —
A combination of wide-angle x-ray solution scattering (WAXS) and neutron spin echo spectroscopy (NSE) was used to probe the structure and dynamics of carbonmonoxy hemoglobin (HbCO) in the presence and absence of the allosteric effector inositol hexaphosphate (IHP). IHP shifts the structure of HbCO slightly towards an unliganded, (deoxy)-state conformation. Two potential binding sites for IHP are consistent with the WAXS data, one near each end of the central channel. IHP binding slows the self-correlation times of some protons, most likely those immediately adjacent to the bound IHP, and simultaneously induces an increase in the relaxation rate of correlated motions with length scales comparable to the $\alpha\beta$-dimer. IHP binding increases the spatial extent of these fluctuations by about 20%. This suggests that when hemoglobin binds CO, its conformation is confined to a relatively narrow structural ensemble residing within a functionally well defined energy well. On the other hand, when it binds both CO and IHP, in response to the contradictory stresses applied by these two ligands, it adopts an incommensurate structure with a conformation exploring a broad structural ensemble.

Jyotsana Lal
Argonne National Laboratory, Argonne IL-60439, USA.

Date submitted: 16 Dec 2010 Electronic form version 1.4