Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Reveal protein dynamics by combining computer simulation and neutron scattering LIANG HONG, JEREMY SMITH, Oak Ridge National Lab, CENTER FOR MOLECULAR BIOPHYSICS TEAM — Protein carries out most functions in living things on the earth through characteristic modulation of its three-dimensional structure over time. Understanding the microscopic nature of the protein internal motion and its connection to the function and structure of the biomolecule is a central topic in biophysics, and of great practical importance for drug design, study of diseases, and the development of renewable energy, etc. Under physiological conditions, protein exhibits a complex dynamics landscape, i.e., a variety of diffusive and conformational motions occur on similar time and length scales. This variety renders difficult the derivation of a simplified description of protein internal motions in terms of a small number of distinct, additive components. This difficulty is overcome by our work using a combined approach of Molecular Dynamics (MD) simulations and the Neutron Scattering experiments [1]. Our approach enables distinct protein motions to be characterized separately, furnishing an in-depth understanding of the connection between protein structure, dynamics and function [2,3].

[1] L. Hong, *et al.*, Phys. Rev. Lett. 107 (2011) 148102.
[2] L. Hong, *et al.*, Phys. Rev. Lett. 108 (2012) 238102.
[3] L. Hong, *et al.*, Phys. Rev. Lett. 110 (2013) 028104.

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Date submitted: 06 Jan 2014 Electronic form version 1.4