Postdoctoral Research Associate in Protein Dynamics

Biosciences Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee

ORNL09-96-BSD

Project Description:
The Biosciences Division at the Oak Ridge National Labortaory is seeking to fill a postdoctoral research position in protein dynamics.

Motions in proteins play a key role in their function. The research here will provide a framework for understanding correlated protein dynamics by combining high-performance simulation with experiments on a next-generation neutron source, the new Spallation Neutron Source at Oak Ridge National Laboratory.

Specifically, we aim to (i) Develop Methodologies will be developed for obtaining simplified descriptions of protein dynamics from computer simulation that are suitable for direct interpretation of dynamic neutron scattering experiments. (ii) Perform experiments and simulations investigating the Pressure Dependence of Protein Dynamics. (iii) Understand the dynamics of protein:protein interactions and correlated intermolecular motions in protein crystals.

An important aspect of the work will be methodological work aimed at obtaining simplified descriptions of protein dynamics from computer simulation that are amenable for direct use in neutron scattering analysis. Transition networks will be constructed describing complex conformational change between known distant conformations as a dense network of subtransitions via low-energy intermediates. Direct analysis of molecular dynamics simulation will be performed in which conformational configurational microstates are merged together in a way that identifies long-lived, i.e., dynamically metastable, states. Dynamics of transitions between metastable states and between transition network nodes will be characterized using a Langevin analysis of the associated coordinate autocorrelation function. Finally, a multiscale, coarse-graining technique based on mapping the atomistic fluctuation covariance matrix onto residue scales modes will be developed. The above methodologies will all be developed, tested, and combined so as to provide an array of possibilities useful for the analysis of a wide range of dynamical phenomena and associated dynamic neutron scattering from biomolecular systems.

Recent simulation work suggests that there is a transition in protein dynamics with pressure at about 4kbar. This transition will be probed experimentally at SNS using backscattering dynamic spectroscopy, and with simulation analysis aimed at identifying the modes responsible for the transition and the role of solvent. Finally, we will examine the dynamics of protein crystals, by measuring inelastic scattering from polycrystalline samples and phonon dispersion relations.

Qualifications:
A Ph.D. in chemistry, physics or computer sciences or closely related field.

Applicants cannot have received the most recent degree more than five years prior to the date of application and must complete all degree requirements before starting their appointment.

Technical Questions:
For more information about this position please contact: Dr. Jeremy C. Smith, Director of the Center for Molecular Biophysics, email: smithjc@ornl.gov or phone: 865-574-9635. Please reference the position title and number when corresponding about this position.

How to Apply:
Qualified applicants may apply online at https://www2.orau.gov/ORNL_POST/. All applicants will need to register before they can begin the online application. For complete instructions, on how to apply, please see the instructions at http://www.orau.gov/orise/edu/ornl/ornl-pdpm/application.htm.

This appointment is offered through the ORNL Postdoctoral Research Associates Program and is administered by Oak Ridge Associated Universities (ORAU). This appointment is open to all qualified U.S. and non-U.S. citizens without regard to race, color, age, religion, sex, national origin, physical or mental disability, or status as a Vietnam-era veteran or disabled veteran.