



UNIVERSITY  
of ARKANSAS  
AT PINE BLUFF  
1873

*Save the Date*

You are all welcome

Department of Chemistry and Physics

Department Seminar

By

Dr. Mahmoud Moradi

Thursday, November 08<sup>th</sup>, 2018

11:00 AM—11:40 AM

STEM BUILDING

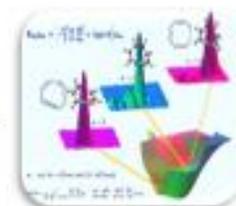
Conference Room



Research Title



- 1) COMPUTATIONAL RECONSTRUCTION OF BIOMOLECULAR PROCESSES.
- 2) SUMMER INTERNSHIP AND GRADUATE SCHOOL PROSPECTS AT UNIVERSITY OF ARKANSAS.



**Department of Chemistry and Biochemistry  
University of Arkansas, Fayetteville**

High-resolution protein structure determination techniques have had various advancements in recent years, encouraging the study of structure-function relationships in proteins. While such techniques provide high-resolution snapshots of protein structure at select functional states, a detailed picture of protein dynamics can be currently produced only using all-atom molecular dynamics simulation technique. Various challenges have, however, hindered the use of molecular dynamics to study the functionally important biomolecular processes such as large-scale conformational changes of proteins. Such functionally important conformational changes often occur on timescales inaccessible to brute-force molecular dynamics. Many enhanced sampling techniques have been developed to address these limitations. However, brute-force molecular dynamics remains the most common method for the computational study of biomolecular systems such as membrane transport proteins. The functionally relevant transitions, on the other hand, are studied using simplistic models. We have been developing methodologies that can characterize the functionally relevant processes in biomolecular systems without compromising the chemical details. These methodologies specifically employ state-of-the-art statistical techniques to enhance the sampling of protein conformational space and use large supercomputing resources to perform ensemble-based molecular dynamics simulations. Several applications will be discussed including the full characterization of transport cycle of a membrane transporter.

**Bio:**

Mahmoud Moradi is an assistant professor at the Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville. He received his B.Sc. and M.Sc. in physics from the Sharif University of Technology in Tehran, Iran. He received his PhD in physics from the North Carolina State University in 2011. He then continued his studies as a postdoctoral fellow at the Beckman Institute, University of Illinois at Urbana-Champaign. He joined the faculty of the Department of Chemistry and Biochemistry at the University of Arkansas, Fayetteville in 2015. He is an editorial board member for Scientific Reports of Nature Publishing Group.