

The Theoretical and Computational Biophysics Group and the  
Center for Multiscale Modeling of Biological Systems present:  
*Hands-on Workshop on Computational Biophysics*



**June 10-14, 2013, Pittsburgh, Pennsylvania**



## The Program

### *Hands-on Workshop in Computational Biology*



Prof. Klaus Schulten



Prof. Emad Tajkhorshid



Prof. Ivet Bahar



Prof. Timothy Lezon



Dr. Ahmet Bakan

Locations at PSC:

Lectures: Room 103

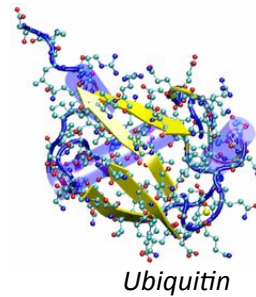
Labs: Room 110



# Mon, 6/10: *Introduction to Protein Structure and Dynamics*



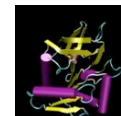
08:00-08:30	<i>Registration and Continental Breakfast</i>
08:30-09:00	Welcome and Brief Overview – Ivet Bahar
09:00-09:10	Opening Remarks
09:10-10:40	Structure and Sequence Analysis with VMD
<i>Break</i>	
11:00-12:00	Introduction to Molecular Dynamics with NAMD
12:00-12:20	Q & A
<i>Lunch</i>	
14:00-16:00	VMD Tutorial - Using VMD; NAMD Tutorial
<i>Break</i>	
16:15-18:00	VMD Tutorial - Using VMD; NAMD Tutorial



# Tue, 6/11: *Statistical Mechanics of Proteins; Force Field Parameterization*



08:30-09:00	<i>Continental breakfast</i>
09:00-10:30	Applications of VMD/NAMD in Modern Research – K. Schulten
<i>Break</i>	
10:50-12:00	Topology, Parameters, and Structure Files – E. Tajkhorshid
12:00-12:30	Q & A; Group photo
<i>Lunch</i>	
14:00-16:00	Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set; Parameterization; Topology Files
<i>Break</i>	
16:15-18:00	Tutorial options: NAMD Tutorial & Stretching Deca-alanine; Expert NAMD Set; Parameterization; Topology Files
<i>Dinner</i>	
19:00-21:00	Participant Presentations

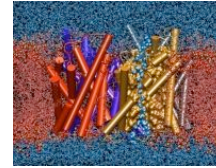


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## Wed, 6/12: *Simulating Membrane Channels*



08:30-9:00	<i>Continental breakfast</i>
09:00-10:30	Introduction and Examples
<i>Break</i>	
10:50-12:00	Transport in Membrane Channels
12:00-12:20	Daily Q&A
<i>Lunch</i>	
14:00-16:00	Tutorial options: Membrane Proteins; Open Tutorial Time
<i>Break</i>	
16:15-18:00	Tutorial options: Membrane Proteins; Open Tutorial Time



*Water Permeation  
through Aquaporin*

## Thu, 6/13: *Collective Dynamics of Proteins Using Elastic Network Models*



08:30-9:00	<i>Continental breakfast</i>
09:00-10:30	Elastic Network Models (ENMs) and Collective Motions of
<i>Break</i>	
10:50-12:00	ProDy Overview and Applications
12:00-12:20	Daily Q&A
<i>Lunch</i>	
14:00-16:00	Tutorial options: ProDy Tutorial; NMWiz Tutorial
<i>Break</i>	
16:15-18:00	Tutorial options: ENM Analysis; Ensemble Analysis; Structure Analysis; Trajectory Analysis; Conformational Sampling

## Thu, 6/14: *Druggability Simulations, and Analyzing Sequence Patterns and Structural Dynamics*



08:30-9:00

*Continental breakfast*

09:00-10:30

Druggability: Method and Applications

*Break*

10:50-12:00

Comparative Analysis of Sequence Patterns and Structural Dynamics for Families/Ensembles of Proteins

12:00-12:20

Daily Q&A

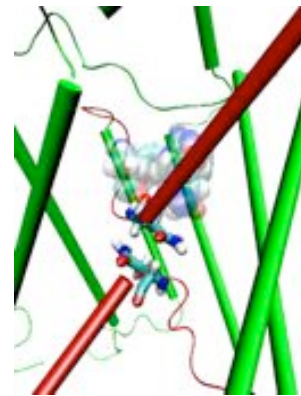
*Lunch*

13:30-15:00

Tutorial options: Druggability Tutorial; Evol Tutorial



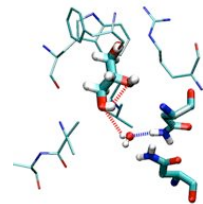
# General



- **The course is a volunteer effort**
- **The main focus are the hands-on sessions**
- **The aim is to get you to do computational biology**
- **The lecturers / teaching assistants provide tutorials for you**
- **The optimal course is that you help each other**

- **Model your own system**

- **Please give us feedback to improve lectures and tutorials**
- **Please give us feedback to encourage future courses**

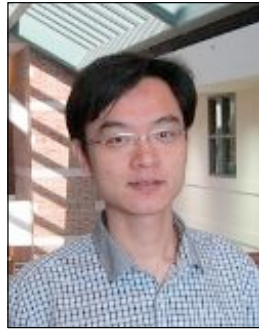


# *Acknowledgements*

## *Teaching Assistants*



Juan Perilla



Wen Ma



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NRBS/PSC