

Beijing Symposium on Protein Folding, Function and Dynamics

Monday July 4

08:30-08:40 Welcome Remarks

Session I Chairman: Feng Gai (UPenn)

08:40-09:40 Michael Levitt (Stanford University)

Using Toys Models to Explore the Protein Universe

09:40-10:15 Ruhong Zhou (IBM/Columbia U)

Dewetting Transition and Hydrophobic Collapse in Protein Aggregates

10:15-10:35 Tea Break

10:35-11:10 Martin Gruebele (UIUC)

Downhill Folding on Rough Free Energy Surfaces: physics and evolution at work

11:10-11:45 Hiroshi Kihara (Kansai Medical U)

Alpha-helix-rich folding core of beta-sheeted proteins

12:00-13:30 Lunch

Session II Chairman: Valerie Daggett (University of Washington)

13:30-14:05 Huanxiang Zhou(Florida State University)

Electrostatic Interactions in Unfolded, Folded, Complexed, and Transition States of Proteins

14:05-14:40 Jianpeng Ma (Baylor/Rice)

New Methods for Simulating Protein Dynamics at Multi-resolution and Multi-length Scales

14:40-15:15 Hue Sun Chan (Toronto U)

Desolvation is a Likely Origin of Robust Enthalpic Barriers to Cooperative Protein Folding

15:15-15:50 Jin Wang (SUNY Stony Brook)

Diffusion Dynamics of Protein Folding

15:50-16:10 Tea Break

Session III Chairman: Yunyu Shi (USTC)

16:10-16:45 Junmei Zhou (Inst. Of Biophysics, CAS)

Molecular Chaperone Function of Escherichia coli Trigger Factor

16:45-17:20 Yi Liang (Wuhan University)

Mixed Macromolecular Crowding Accelerates the Oxidative Refolding of Reduced, Denatured Lysozyme: Implications for Protein Folding in Intracellular Environments

17:20-17:55 Changwen Jin (PKU)

Solution Structures and Functional Insights of an Arsenate Reductase from Bacillus subtilis: Reversible Conformational Switch Associates with the Arsenate Reduction

Tuesday, July 5

Session I Chairman: Jeff Saven (UPenn)

08:30-09:30 Alan Fersht (Cambridge University)

How Small Proteins Fold

09:30-10:05 Yunyu Shi (USTC)

Protein structure and protein-protein interaction studied by NMR

10:05-10:25 Tea Break

10:25-11:00 Valerie Daggett (University of Washington)

Protein Unfolding and Refolding at Atomic Resolution

11:00-11:35 Yong Duan (UC Davis)

Folding and aggregation: A physics-based all-atom modeling

11:35-11:50 Sarah Perrett (Inst. Of Biophysics, CAS)

Factors influencing the function, folding and fibril formation of the yeast prion protein ure2

12:00-13:30 Lunch

Session II Chairman: Chih-Chen Wang (Inst. Of Biophysics, CAS)

13:30-14:05 Feng Gai (UPenn)

Understanding the Folding Mechanism of β -Hairpins

14:05-14:40 Yongzhang Luo (Tsinghua U)

Refolding of Proteins from in vitro to in vivo

14:40-15:15 Zengyi Chang (PKU)

Immediate response to stress conditions for the structure and activity of molecular Chaperones

15:15-15:50 Chi-Ming Chen (National Taiwan Normal University, Taiwan)

Structure Prediction and Folding Dynamics of Bacteriorhodopsin

15:50-16:10 Tea Break

Session III Chairman: Luhua Lai (PKU)

16:10-16:25 Yuguang Mu (Nanyang Technological University, Singapore; ShanDong University, China)

Intermediate states of forming binding protein WW domain: explored by replica-exchange simulation

16:25-16:40 Fan Jiang (Institute of Physics, CAS)

Scaling laws in folding of native protein structures

16:40-16:55 Bin Lai (Stony Brook University)

Translocation of Diphtheria Toxin T Domain-Induced Translocation of the Diphtheria Toxin Catalytic Domain (A Chain) Across Membranes: Role of Changes in Protein Folding/Unfolding

16:55-17:10 Rongzheng Wan (Shanghai Institute of Applied Physics, CAS)

Controllable water channel gating of nanometer dimensions

17:10-17:25 Ming Lei (Beijing University of Chemical Technology)

Role of conformational change in initial partial disrupted path of V14N/V16E mutant of transthyretin: Insights from molecular dynamic simulation

17:25-17:40 Xiaohong Shi (Huazhong University of Sciences and Technology)

A Finding Maximal Clique Algorithm for predicting Loop of Protein Structure

17:40-17:55 Ying-Chieh Sun(National Taiwan Normal University, Taiwan)

Examination of Several Factors Affecting Folding of Short Helical Peptides Using Molecular Dynamics Simulation

Wednesday July 6

Session I Chairman: Zengyi Chang (PKU)

08:30-09:30 Chih-Chen Wang (Inst. Of Biophysics, CAS)

Dimerization and chaperone activity of thiol-protein oxidoreductases

09:30-10:05 Yawen Bai (NIH)

Hidden Intermediates at Atomic Resolution: Implications for Protein Folding

10:05-10:25 Tea Break

10:25-11:00 Wei Wang (Nanjing U)

Folding of small proteins using simplified Go-model and all-atom model

11:00-11:35 Emily Ching (Chinese U of HK)

Characteristic patterns in amino acid sequences and their use in the

prediction of protein structures

11:35-11:50 Aoneng Cao (PKU)

Mechanism of the folding and chaperone-like activity of the small heat shock protein from *Methanococcus jannaschii*

12:00-13:30 Lunch

13:30-15:00 Poster Session

Tuesday July 7

Session I Chairman: Ruhong Zhou (IBM/Columbia U)

08:30-09:30 William Degrado (UPenn)

De Novo design of Catalytic Proteins

09:30-10:05 Chao Tang (UCSF/PKU)

Flexibility of secondary structures from database analysis

10:05-10:25 Tea Break

10:25-11:00 Yaoqi Zhou (SUNY Buffalo)

Molecular mechanism of binding cooperativity in a dimeric hemoglobin

11:00-11:35 Ray Luo (UC Irvine)

Unfolding and refolding of p53 cancer and suppressor mutations

11:35-11:50 Jingyuan Li (Zhejiang University)

Hydration and Dewetting near Graphite-CH₃ and Graphite-COOH Plates

12:00-13:30 Lunch

Session II Chairman: Chao Tang (UCSF/PKU)

13:30-14:05 Jeff Saven (UPenn)

Methods for engineering protein structure and function with computational protein design

14:05-14:40 Chen Zeng (George Washington U)

Application of Generic Sidechains and Softmodes in Protein Design

14:40-15:15 Hong Qian (U. of Washington)

Dynamics on Energy Landscapes: From Protein Folding Pathways to Open-systems Thermodynamics of Kinetic Proofreading

15:15-15:50 Luhua Lai (PKU)

Functional Protein Design Targeting Protein-Protein Interface