

THE ROLE OF FLUCTUATIONS AND DYNAMICS IN BIOMOLECULAR FUNCTION

7-11 JANUARY 2019

TELLURIDE SCIENCE RESEARCH CENTER
The Depot and Aa Haa School for the Arts
300 S. Townsend Street, Telluride, CO 81435

Sunday 6:00-7:30 PM

6:00PM Registration and welcome reception
The Phoenix Bean, 221 W. Colorado Avenue

Monday 8:00-9:00 AM

8:00 AM Breakfast @ The Depot

Monday 3:15-6:15 PM (three talks)

3:15 PM Introductory remarks
3:30 PM Markus MEUWLY
Structural interpretations of time scales from atomistic simulations
4:15 PM Norio YOSHIDA
pKa prediction of titratable residues in protein
5:00 PM Coffee Break
5:30 PM Pratyush TIWARY
All-atom modeling of biomolecular rare events with statistical mechanics and artificial intelligence
7:00 PM Dinner
Sideworks, 225 S. Pine Street

Tuesday 8:00-11:15 AM (three talks)

8:00 AM Breakfast
8:30 AM Dmitry MATYUSHOV
Fluctuations of protein and water in enzyme catalysis
9:15 AM Akio KITAO
Simulating dissociation and association processes of protein complexes
10:00 AM Coffee Break
10:30 AM Masatake SUGITA
Exploring the ligand binding mode on a fluctuating protein

Tuesday 4:45-6:15 PM (two talks)

4:45 PM Rigoberto HERNANDEZ
Dynamical Consistency in Sustainable Nanoparticles
5:30 PM Fumio HIRATA
Structural fluctuation of protein and Anfinsen's dogma
7:00 PM Dinner (free)

Wednesday 8:00-11:15 AM (three talks)

8:00 AM Breakfast
8:30 AM David LEITNER
Relations between protein-water equilibrium dynamics and energy transfer kinetics
9:15 AM Taka YAMATO
Energy transfer and residue interaction network of proteins

10:00 AM Coffee Break
10:30 AM Matthias HEYDEN
Fluctuations of protein hydration

Wednesday 4:45-6:15 PM (two talks)

4:45 PM Yuko OKAMOTO
Enhanced sampling techniques to study fluctuations and dynamics in molecular systems
5:30 PM Changbong HYEON
Energetic cost, speed, fluctuations, and transport efficiency of biological motors
7:00 PM Dinner (free)

Thursday 8:00–11:15 AM (three talks)

8:00 AM Breakfast
8:30 AM Qiang CUI
Water, fluctuations and protein allostery
9:15 AM Ayori MITSUTAKE
Analysis for stability and dynamics of protein folding with methods based on statistical mechanics
10:00 AM Coffee Break
10:30 AM Ryo AKIYAMA
Effective attraction between negatively charged patches on protein in an electrolyte solution

Thursday 4:45-6:15 PM (two talks)

4:45 PM John STRAUB
Probing the rules governing domain formation and protein partitioning in membrane
5:30 PM Masataka NAGAOKA
TBA
7:00 PM Dinner
The Chop House, 233 W. Colorado Avenue

Friday 8:00–11:00 AM (open discussion)

8:00 AM Breakfast
8:30 AM Open discussion and concluding remarks
11:00 AM Adjourn