PROGRAM

**Telluride Science Research Center**

**Workshop on Protein Dynamics**

**July 30 – August 4, 2017**



***Organizers:***

Paul Fenimore Los Alamos National Laboratory

Rafael Brüschweiler The Ohio State University

Takayuki Nishizaka Gakushuin University

***TSRC office:***

Mark Kozak mark@telluridescience.org / +1 970 708 4426

***Location of the meeting and breakfast:***

Telluride Intermediate School 725 West Colorado Ave, Telluride

**Participants**

* Anfinrud, Philip - National Institutes of Health (USA)
* Blackledge, Martin - Institut de Biologie Structurale (FR)
* Brüschweiler, Rafael - Ohio State University (USA)
* Fenimore, Paul - Los Alamos National Laboratory (USA)
* Fonseca, Rasmus – Stanford University (USA)
* Frauenfelder, Hans - Los Alamos National Laboratory (USA)
* Havenith, Martina - Bochum University (DE)
* Hayashi, Shigehiko – Kyoto University (JP)
* Head-Gordon, Teresa – University of California, Berkeley (USA)
* Kitao, Akio - The University of Tokyo (JP)
* Lindorff-Larsen, Kresten - Copenhagen University (DK)
* Nishizaka, Takayuki - Gakushuin University (JP)
* McDermott, Ann - Columbia University (USA)
* Meuwly, Markus – University of Basel (CH)
* Mizutani, Yasuhisa - Osaka University (JP)
* Oroguchi, Tomotaka - Keio University (JP)
* Palmer, Arthur - Columbia University (USA)
* Sage, J Timothy - Northeastern University (USA)
* Straub, John - Boston University (USA)
* Thielges, Megan – Indiana University (USA)
* Tobias, Doug – University of California, Irvine (USA)
* Uchihashi, Takayuki – University of Kanazawa (JP)
* van Thor, Jasper - Imperial College London (UK)
* Weik, Martin - Institut de Biologie Structurale (FR)
* Yamato, Takahisa - Nagoya University (JP)

**Sunday, July 30**

**14:00-17:00** Summer School Mini-Symposium: Rm. 224 Intermediate School

Biomolecular Structure and Dynamics: Theory and Experiment

**17:00** Reception: Telluride Intermediate School, Eastside tent

**Monday, July 31**

**8:00-8:20** Breakfast

**8:20-8:30** Welcome

Session Chair: Paul Fenimore

**8:30-9:15 Tobias, Doug**

Simulation studies of protein interactions, organization, and dynamics in crowded solutions

**9:15-10:00 Kitao, Akio**

 Dissociation and association dynamics of proteins

**10:00-10:30** Break

**10:30-11:15 Thielges, Megan**

 Dynamics of protein molecular recognition by 2D IR spectroscopy

**11:15-12:00 McDermott, Ann**

 The signaling complex in necroptosis is a structurally novel amyloid

*Lunch break*

Session Chair: Rafael Brüschweiler

**14:30-15:15 Havenith, Martina**

Water mapping by THz calorimetry

**15:15-16:00 Oruguchi, Tomotaka**

 Protein conformational fluctuations and hydration structures investigated by the combination of MD simulations and X-ray experiments

**16:00-16:45 Fenimore, Paul**

 Hydration water structures

**Tuesday, August 1st**

Session Chair: Takayuki Nishizaki

**12:00-12:45 Brüschweiler, Rafael**

 Dynamics of function-critical protein states: enzymes, loops, and IDPs

**12:45-13:30 Head-Gordon, Teresa**

 Statistical fluctuations, dynamics, scaffolds, electric fields, and *de novo* enzyme catalysis

**13:30-14:00** Break

**14:00-14:45 Lindorff-Larsen, Kresten**

 From protein folding to patient diagnosis

**14:45-15:30 Blackledge, Martin**

 Large scale protein dynamics - from fundamental biophysics and biological function

**15:30-15:50** Break

**15:50-16:35 Palmer, Arthur**

Spin relaxation in proteins: methods and applications

**16:35-17:20 Mizutani, Yashuhisa**

 Importance of atomic contacts to propagations in protein: functional compactness

**18:00-19:00** Town Talk at the Conference Center in Mountain Village.

Allow 35 minutes to travel there. Cash bar opens at 17:30.

**Wednesday, August 2nd**

**8:00-8:30** Breakfast

Session Chair: Doug Tobias

**8:30-9:15 Anfinrud, Phil**

 Time-resolved x-ray and NMR studies of biomolecules: from folding to function

**9:15-10:00 Uchihashi, Takayuki**

 Direct visualization of single molecule dynamics by high-speed atomic force microscopy

**10:00-10:30** Break

**10:30-11:15 Nishizaki, Takayuki**

 Development of imaging techniques to reveal single-protein dynamics and their application to microbiology

**11:15-12:00 Weik, Martin**

 Time-resolved serial femtosecond crystallography on photoswitchable fluorescent proteins

*Lunch break*

Session Chair: Martina Havenith

**14:30-15:15 Frauenfelder, Hans**

 The spatial diffusion and the energy landscape model for thermal neutron scattering

**15:15-16:00 Sage, Timothy**

Influence of vibrational and supravibrational dynamics on nuclear resonance absorption

**16:00-16:30** Break

**16:30-17:15 Fonseca, Rasmus**

 Efficient conformational interpretation of DEER using structural and dynamic constraints

**17:15-18:00 Meuwly, Markus**

 Protein metastable states from atomistic simulations

**18:00-20:00** Picnic at the Telluride Intermediate School

**Thursday, August 3**

Session Chair: Phil Anfinrud

**14:30-15:15 van Thor, Jasper**

 Approaches to study exciton dynamics and charge separation in photosynthesis

**15:15-16:00 Yamato, Takahisa**

 Forced unfolding mechanism of bacteriorhodopsin as revealed by coarse-grained molecular dynamics

**16:00-16:30** Break

**16:30-17:15 Hayashi, Shigehiko**

 Understanding and Designing Color Variants of Retinal Binding Proteins by Molecular Simulations

**17:15-18:00 Straub, John**

 The role of lipid composition, domains, and interfaces in membrane protein structure and function

**18:00-19:45** Casual dinner at the school will be arranged and business meeting. TBA during the workshop with participants.

**19:45-20:00** Closing remarks