Program of the 2014 Les Houches - TSRC Workshop on Protein Dynamics

Monday, May 19, 2014	
7:45 – 8:30	Breakfast
8:30 - 9:00	Welcome and introductory remarks
	Martin Weik (IBS Grenoble) and Nana Naisbitt (TSRC)
9:00 – 12:30	Protein dynamics from x-ray scattering I
	Discussion Leader: Jasper van Thor
9:00 – 9:45	Thomas BARENDS (MPI Heidelberg) PROTEIN CRYSTALLOGRAPHY WITH X-RAY FREE-ELECTRON LASERS
9:45 – 10:30	James FRASER (UC San Francisco) E PLURIBUS UNUM, NO MORE: FROM ONE CRYSTAL, MANY CONFORMATIONS
10:30 - 11:00	Break
11:00 – 11:45	Marco CAMMARATA (University of Rennes) PROTEIN STRUCTURAL DYNAMICS VIA (TIME-RESOLVED) WIDE ANGLE X-RAY SCATTERING
11:45 – 12:30	Arwen PEARSON (DESY Hamburg) NEW DATA COLLECTION STRATEGIES FOR TIME-RESOLVED EXPERIMENTS
12:30 - 14:00	Lunch
14:30 – 16:00	New experimental and simulation approaches I Discussion Leader: Tamiki Komatsuzaki
14:30 – 15:15	Daria KOKH (HITS Heidelberg) STUDY OF SLOW CONFORMATIONAL CHANGES IN PROTEINS
15:15 – 16:00	Minhaeng CHO (Korea University) AMPLIFICATIONS IN COHERENT CHIROPTICAL SPECTROSCOPY AND QUANTUM WEAK MEASUREMENT
16:00 - 16:30	Break
16:30 - 18:00	Correlated protein-solvent dynamics
	Discussion Leader: David Leitner
16:30 – 17:15	Martina HAVENITH (Bochum University) SOME LIKE IT COOL – THZ ABSORPTION STUDIES OF AS A TOOL TO STUDY BIOMOLECULAR HYDRATION
17:15 – 18:00	Matthias HEYDEN (MPI Mühlheim) CORRELATIONS IN PROTEIN AND SOLVENT DYNAMICS STUDIED WITH ATOMISTIC MOLECULAR DYNAMICS SIMULATIONS
18:00 - 19:00	Poster clips
	Chair: Nana Naisbitt
19:30 - 21:00	Dinner

Tuesday, May 20, 2014		
7:45 – 8:45	Breakfast	
8:45 – 10:15	NMR studies of protein dynamics I	
8:45 – 9:30	Paul SCHANDA (IBS Grenoble) SOLID-STATE NMR: NEW INSIGHT INTO DYNAMICS IN CRYSTALLINE PROTEINS AND LARGE MOLECULAR ASSEMBLIES	
9:30 – 10:15	Frans MULDER (Aarhus University) NMR SPECTROSCOPIC INVESTIGATION OF THE PH-DEPENDENT PHOTOCYCLE DYNAMICS OF PHOTOACTIVE YELLOW PROTEIN	
10:15 – 10:45	Break	
10:45 – 12:15	Enzyme catalysis Discussion Leader: James Fraser	
10:45 – 11:30	Martin FIELD (IBS Grenoble) MOLECULAR SIMULATIONS OF ENZYME CATALYSIS	
11:30 – 12:15	Shigehiko HAYASHI (Kyoto University) CRUCIAL ROLE OF PROTEIN FLEXIBILITY IN ENZYMATIC CATALYSIS	
12:30 – 14:00	Lunch	
14:00 - 19:30	Free Time	
19:30 – 21:00	Dinner	

Wednesday, May 21, 2014		
7:45 – 8:45	Breakfast	
8:45 – 10:15	Protein dynamics from x-ray scattering II Discussion Leader: Arwen Pearson	
8:45 – 9:30	Junko YANO (Lawrence Berkeley National Laboratory, Berkeley) WATER OXIDATION REACTION CATALYZED BY THE MN4CAO5 CLUSTER IN PHOTOSYSTEM II	
9:30 – 10:15	Jasper van THOR (Imperial College London) SIGNAL TO NOISE CONSIDERATIONS FOR SINGLE CRYSTAL FEMTOSECOND TIME RESOLVED CRSYTALLOGRAPHY OF PHOTOACTIVE YELLOW PROTEIN	
10:15 - 10:45	Break	
10:45 – 12:15	New experimental and simulation approaches II Discussion Leader: Minhaeng Cho	
10:45 – 11:30	Tamiki KOMATSUZAKI (Hokkaido University) ENERGY LANDSCAPES CONSTRUCTED FROM SINGLE-MOLECULE TIME SERIES AND REACTION NETWORKS	
11:30 – 12:15	Andrea MARKELZ (University at Buffalo) PROTEIN PICOSECOND CORRELATED MOTIONS AND DYNAMICAL ENSEMBLE ACCESS	
12:30 - 14:00	Lunch	
14:30 – 18:00	Membrane proteins and protein aggregation Discussion Leader: John Straub	
14:30 – 15:15	Mounir TAREK (Université de Lorraine, Nancy) MODULATION OF VOLTAGE GATED ION CHANNELS BY LIPIDS	
15:15 – 16:00	Simon SCHEURING (Aix-Marseille Université) HIGH-SPEED ATOMIC FORCE MICROSCOPY MONITORS MEMBRANE PROTEIN DYNAMICS	
16:00 – 16:30	Break	
16:30 – 17:15	Joan-Emma SHEA (UC Santa Barbara) EFFECT OF SURFACES IN MODULATING PROTEIN FOLDING AND AGGREGATION MECHANISMS	
17:15 – 18:00	Birgit STRODEL (Forschungszentrum Juelich) KINETICS OF AMYLOID BETA-PROTEIN AGGREGATION IN THE ABSENCE/PRESENCE OF FIBRILS	
18:00 - 19:30	Poster session	
19:30 - 21:00	Dinner	

	Thursday, May 22, 2014
7:45 – 8:45	Breakfast
8:45 – 12:30	Free Time
12:30 – 14:00	Lunch
14:30 – 16:45	Energy, heat, and signal flow in proteins Discussion Leader: Paul Champion
14:30 – 15:15	Peter HAMM (University Zurich) DYNAMICS OF A PHOTOSWITCHABLE ALLOSTERIC PROTEIN
15:15 – 16:00	Gerhard STOCK (University of Freiburg) ENERGY AND SIGNAL FLOW IN BIOMOLECULES
16:00 – 16:45	David LEITNER (University of Nevada at Reno) ENERGY TRANSFER AT THE PROTEIN-WATER INTERFACE AND THERMAL CONDUCTIVITY OF THE CELL
16:45 – 17:15	Break
17:15 – 18:45	Protein dynamics from neutron scattering Discussion Leader: Martin Weik
17:15 – 18:00	Alessandro PACIARONI (University of Perugia) PROTEIN DYNAMICS IN THE HIGH TEMPERATURE RANGE: CRITICAL FLUCTUATIONS AT THERMAL MELTING
18:00 – 18:45	Joe ZACCAI (Institut Laue Langevin, Grenoble) 'VISUALIZING' STRUCTURE, DYNAMICS AND FUNCTIONAL INTERACTIONS OF BIOLOGICAL MOLECULES BY NEUTRON SCATTERING
19:30 - 21:00	Dinner

Friday, May 23, 2014	
7:45 – 8:45	Breakfast
8:45 – 10:15	Electron and proton transfer in proteins Discussion Leader: Martin Field
8:45 – 9:30	Ana-Nicoleta BONDAR (Freie Universität Berlin) WATER AND HYDROGEN BOND DYNAMICS IN PROTON-TRANSFER SYSTEMS
9:30 – 10:15	Paul CHAMPION (Northeastern University, Boston) PROBING LOW FREQUENCY VIBRATIONAL EXCITATIONS AND THEIR EFFECT ON ELECTRON AND PROTON TRANSPORT IN PROTEINS
10:15 - 10:45	Break
10:45 – 12:15	NMR studies of protein dynamics II Discussion Leader: Douglas Tobias
10:45 – 11:30	Joshua WAND (University of Pennsylvania) THE DARK ENERGY OF PROTEINS COMES TO LIGHT: CONFORMATIONAL ENTROPY IN PROTEIN FUNCTION
11:30 – 12:15	Martin BLACKLEDGE (IBS, Grenoble) NMR STUDIES OF PROTEIN MOTIONS ON MULTIPLE TIMESCALES – FROM FUNDAMENTAL BIOPHYSICS TO FUNCTIONAL DYNAMICS
12:15 – 12:30	<i>Closing remarks</i> John Straub (Boston University) and Douglas Tobias (UC Irvine)
12:30 - 14:00	Lunch and Departure