



Martin Karplus Celebration Symposium

HOME

PROGRAM

SHORT TALKS

REGISTRATION

LODGING

INFO

SPONSORS

Short Talks

September 30th, 2014, Helen Diller HD 160, [UCSF Cancer Center, 1450 3rd St, San Francisco, CA 94158, San Francisco](#)
 (The [Symposium](#) will be held at a different location - [The Mark Hopkins Hotel, 999 California St., San Francisco](#))

Tuesday, September 30th - 12-5 pm

12:00-12:10	<u>Moderator</u>	Andrej Sali	University of California, San Francisco, USA
12:10-12:25	QM/MM investigation of substrate-assisted catalysis	Hong Guo	University of Tennessee
12:25-12:40	An overview of simulations on the plexin and Eph transmembrane receptor systems	Matthias Buck	Case Western Reserve
12:40-12:55	How insulin binds: from structure of a model hormone-receptor complex to next-generation analog design	Michael Weiss	Case Western Reserve
12:55-1:10	Substrate-Assisted Glycosylation Reaction Follows a Highly Concerted Pathway that Leads to a Low-Barrier-Hydrogen-Bond Transition State	Wei Yang	Florida State University
1:10-1:25	Binding mechanism of intrinsically disordered proteins from molecular simulation	Robert Best	NIDDK, National Institutes of Health
1:25-1:40	On the Question of Atoms and Bonds in Molecules	Peter Langhoff	UC San Diego
1:40-1:55	Toward understanding the ATP hydrolysis mechanism in ABC-transporters: insights from multiscale simulations	Jingzhi Pu	Indiana University-Purdue University
1:55-2:10	Ab initio dynamics of proteins by using FMO	Yuri Alexeev	Argonne National Laboratory
2:10-2:25	Reactions at water surfaces: aerosols, vesicles and bubbles	Veronica Vaida	University of Colorado, Boulder
2:25-2:55	BREAK		
	<u>Moderator</u>	Matt Jacobson	University of California, San Francisco, USA
2:55-3:10	Simulating biomolecular processes at multiple scales	Wonmuk Hwang	Texas A&M University
3:10-3:25	Multi-scale QM/MM model for the study of catalytic mechanism of protein tyrosine kinase	Kwangho Nam	Umea University
3:25-3:40	Multiscale Motions in Nucleic Acids	Ioan Andricioaei	UC Irvine
3:40-3:55	The SCOPe database (http://scop.berkeley.edu)	John-Marc Chandonia	Berkeley National Lab
3:55-4:10	Uncovering the complex pathway of helix formation	Krzysztof Kuczera	University of Kansas
4:10-4:25	Protein Electrodynamics and Terahertz Medicine	Ogan Gurel	Samsung Advanced Institute of Technology
4:25-4:40	Ras GTPase: Effects of oncogenic mutants	Carla Mattos	Northeastern University

--	--