Martin Karplus
Celebration Symposium

October 1, 2014

On computational methods applied to chemical and biological systems

The Mark Hopkins Hotel, 999 California Street, San Francisco, CA, USA

Preface

This symposium recognizes the scientific accomplishments of Martin Karplus and his students. It also celebrates Martin's receipt of the 2013 Nobel Prize in Chemistry for the development of multiscale models for complex chemical systems. Driven by a desire to discover new things and to understand biological processes at a fundamental level in chemical and physical terms, Martin has contributed in inestimable ways to the field of theoretical chemistry and to the development of molecular dynamics simulation of biomolecules. Early on, Martin concentrated on chemical physics and provided critical insights on topics including magnetic resonance and dynamics of fundamental reactions like H + H_2. At Harvard, he charted a new path that directed his efforts to biology, thus returning to what first attracted him to science as a young boy. As well as his own scientific work, Martin's contributions include his influence on the nearly 250 students and postdocs who have been members of his research group. He provided an environment with highest scientific standards and a need for rigorous, critical thinking. This symposium is the third such gathering to bring together past group members to meet, discuss, and this year, to celebrate together the well deserved Nobel Prize.

Karplusians : 1955-2014

Ivana Adamovic
Yuri Alexeev
David H. Anderson
Ioan Andricioaei
Yasuhide Arata
Georgios Archontis
Gabriel G. Balint-Kurti
Christian Bartels
Paul Bash
Donald Bashford
Mark Bathe
Oren M. Becker
Robert Best
Anton Beyer
Robert Birge
Ryan Bitetti-Putzer
Arnaud Blondel
Stefan Boresch
John Brady
Bernard Brooks
Charles L. Brooks III
Thomas H. Brown
Robert E. Bruccoleri
Paul W. Brumer
Axel T. Brünger
Rafael P. Brüschweiler
Matthias Buck
Amedeo Caflisch
William J. Campion
William Carlson
David A. Case
Leo Caves
Thomas C. Caves
Marco Cecchini
John-Marc Chandonia
Ta-Yuan Chang
Xavier Chapuisat
Sergei Chekmarev
Rob D. Coalson
François Colonna-Cesari
Michael R. Cook
Qiang Cui
Tara Prasad Das
Annick Dejaegere
Philippe Derreumaux
Aaron Dinner
Uri Dinur
Roland L. Dunbrack, Jr.
Chizuko Dutta
Nader Dutta
Claus Ehrhardt
Ron Elber
Marcus Elstner
Byung Chan Eu
Jeffrey Evanseck
Erik Evensen
Jeffrey Evenson
Thomas C. Farrar
Martin J. Field
Stefan Fischer
David L. Freeman
Thomas Frimurer
Kevin Gaffney
Jiali Gao
Yi Qin Gao
Bruce Gelin
R. Benny Gerber
Paula M. Getzin
Debra A. Giammona
Martin Godfrey
Andrei Golosov
David M. Grant
Daniel Grell
Peter Grootenhuis
Hong Guo
Ogan Gurel
Robert Harris
Karen Haydock
Russell J. Hemley
Jeffrey C. Hoch
Milan Hodoscek
Gary G. Hoffman
L. Howard Holley
Barry Honig
Victor Hruby
Rod E. Hubbard
Robert P. Hurst
Vincent B.-H. Huynh
Toshiko Ichiye
K. K. Irikura
Alfonso Jaramillo
Tom Jordan
Diane Joseph-McCarthy
Sun-Hee Jung
C. William Kern
William Kirchhoff
Burton S. Kleinman
Gearld W. Koeppl
H. Jerrold Kolker
Yifei Kong
Lewis M. Koppel
J. Kottalam
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Kwango Nam
Eyal Neria
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Dzung Nguyen
Iwao Ohmine
Barry Olafson
Kenneth W. Olsen
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Victor Ovchinnikov
Emanuele Paci
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C.S. Pangali
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Robert Petrella
B. Montgomery Pettitt
Ulrich Pezzeca
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Jay M. Portnow
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Martine Prévost
Blaise Prod'hom
Jingzhi Pu
Dagnija Lazdins Purins
Lionel M. Raff
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Bruno Robert
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Michael Schlenkrich
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Klaus Schulten
Eugene Shakhnovich
Moshe Shapiro
Ramesh D. Sharma
Isaiah Shavitt
Henry H.-L. Shih
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Yudong Wu
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Wei Yang
Robert Yelle
Darrin York
Hsiang-ai Yu
Guishan Zheng
Yaoqi Zhou
Vincent Zoete

Program

Wednesday, October 1, 2014

The Mark Hopkins Hotel, 999 California Street, San Francisco

7:30 - 8:55 AM	Registration and Breakfast *Location: Peacock Court*
8:55 - 9:00 AM	**Andrej Sali,** University of California, San Francisco, CA, USA Welcome Remarks *Location: Room of the Dons*
	Chair **Toshiko Ichiye,** Georgetown University, Washington, DC, USA
9:00 - 9:25 AM	**Andy McCammon**, University of California, San Diego, CA, USA Molecular Dynamics and Drug Discovery
9:25 - 9:55 AM	**Peter Rossky**, University of Texas, Austin, TX, USA *Back to the Future: QM/MM Simulation of Exciton Dynamics in Conjugated Molecular Materials*
9:55 - 10:25 AM	**Iwao Ohmine,** Institute for Molecular Science, Okazaki, Japan *Water Dynamics; fluctuation, phase transitions and reactions*
10:25 - 10:45 AM	Coffee break
	Chair **Tom Simonson,** Ecole Polytechnique, Palaiseau, France
10:45 - 11:15 AM	**Adrian Mulholland,** University of Bristol, Bristol, UK *Enzyme catalytic mechanisms from combined quantum mechanics/molecular mechanics (QM/MM) modeling*
11:15-11:45 AM	**Marco Cecchini,** Université de Strasbourg, France *Computational approaches to chemomechanical transduction: the myosin molecular motor*
11:45 -12:15 PM	**Bernard R. Brooks,** National Institutes of Health, Bethesda, MD, USA *35 years of CHARMM*
12:15 - 1:40 PM	Lunch *Location: Peacock Court*

	Chair **Amedeo Caflisch,** University of Zurich, Switzerland
1:40 - 2:10 PM	**YiQin Gao,** Peking University, Beijing, P.R. China *DNA allostery and its sequence dependence*
2:10 - 2:40 PM	**Collin Stultz,** Massachusetts Institute of Technology, Cambridge, MA, USA *Modeling Intrinsically Disordered Proteins: Application to Amyloid-beta*
2:40 - 3:10 PM	**Paul Maragakis,** DE Shaw Research, New York, NY, USA *Targeting "undruggable" proteins using long molecular dynamics simulations*
3:10 - 3:30 PM	Coffee break
	Chair **John E. Straub,** Boston University, Boston, MA, USA
3:30 - 4:00 PM	**Carol B. Post,** Purdue University, West Lafayette, IN, USA *New structural features of kinases as potential targets to alter protein-protein interactions*
4:00 - 4:30 PM	**Dennis Vitkup,** Columbia University, New York, NY, USA *Systems Biology of Psychiatric Disorders*
4:30 - 5:00 PM	**Axel Brunger,** Stanford University, Stanford, CA, USA *Molecular mechanisms of SNARE-mediated membrane fusion, calcium triggering, and recycling*
5:00 - 5:15 PM	Summing up **David Chandler,** University of California, Berkeley, CA, USA
6:15 - 7:30 PM	Reception *Location: Room of the Dons*
7:30 - 10:00 PM	Dinner *Location: Peacock Court*
	Moderator **John Kuriyan,** University of California, Berkeley, CA, USA
9:10 - 10:00 PM	Address **Greg Petsko,** Weill Cornell Medical School, New York, NY, USA

Short Talks

Tuesday, September 30, 2014

Helen Diller HD 160, UCSF Cancer Center, 3rd Street, San Francisco, CA 94158

12:00 - 5:00 PM

Name	Title
Ogan Gurel	*Protein Electrodynamics and Terahertz Medicine*
Matthias Buck	*An overview of simulations on the plexin and Eph transmembrane receptor systems.*
Michael Weiss	*How insulin binds: from structure of a model hormone-receptor complex to next- generation analog design.*
Wei Yang	*Predictive Sampling of Protein Long-Timescale Motions*
Robert Best	*Binding mechanism of intrinsically disordered proteins from molecular simulation*
Peter Langhoff	*On the Question of Atoms and Bonds in Molecules*
Carla Mattos	*Ras GTPase: Effects of oncogenic mutants*
Yuri Alekseev	*Ab initio dynamics of proteins by using FMO*
Veronica Vaida	*Reactions at water surfaces: aerosols, vesicles and bubbles*
Wonmuk Hwang	*Simulating biomolecular processes at multiple scales*
Kwangho Nam	*Multi-scale QM/MM model for the study of catalytic mechanisms of protein tyrosine kinase*
Ioan Andricioaei	*Multiscale Motions in Nucleic Acids*
John-Marc Chandonia	*The SCOPe database (http://scop.berkeley.edu)*
Kryzsztof Kuczera	*Uncovering the complex pathway of helix formation*
Hon Guo	*QM/MM investigation of substrate-assisted catalysis*
Jingzhi Pu	*How ABC-transporters hydrolyze ATP: development and application of QM/MM methods*

Symposium Organizing Committee

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David Chandler, University of California, Berkeley
Matt Jacobson, University of California, San Francisco
John Kuriyan, University of California, Berkeley
Susan Marqusee, University of California, Berkeley
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