Simons Symposium:
Challenges in Biomolecular Simulations

May 6-8, 2024

Contents

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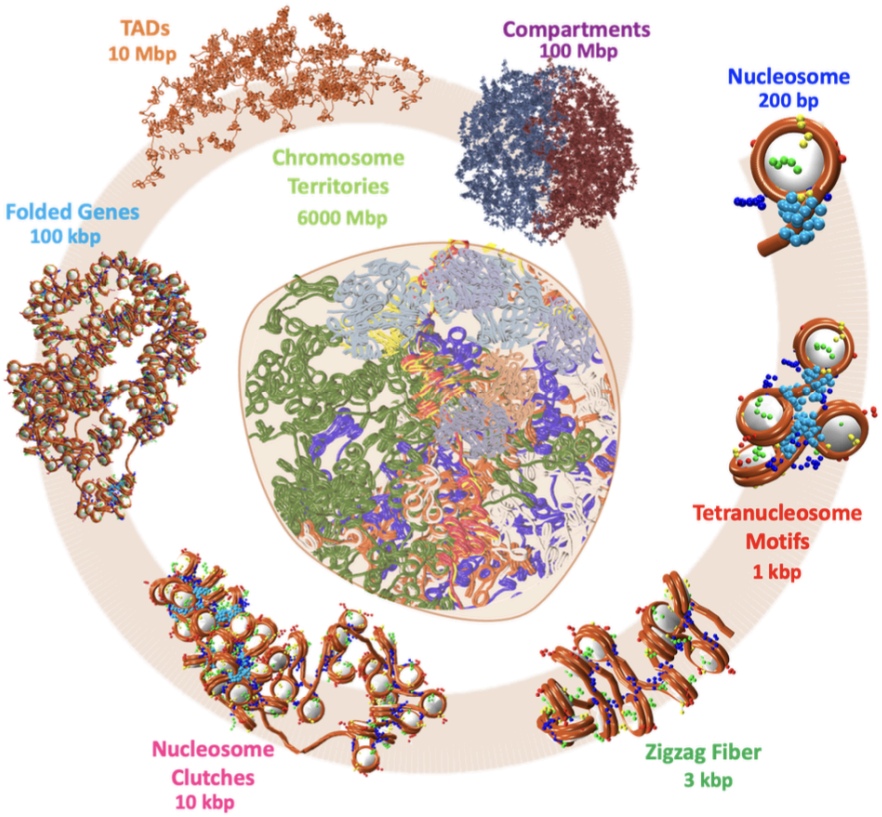
Monday, May 6

Program
Kimmel Center, Shorin 802

Keynote Talk: 25 min + 10 min Q&A
Short Talk: 10 min + 2 min Q&A

9:30 am	Check-in, Continental Breakfast
Session Ia	**Tamar Schlick, NYU, Chair**
10:00 am	Welcoming Remarks: Antonio Merlo, Dean of Arts and Science, New York University
10:10 am	J. Andrew McCammon, University of California, San Diego *Protein Dynamics Zoo: Gating and Channeling*
10:35 am	*Q&A*
10:45 am	Emad Tajkhorshid, University of Illinois at Urbana-Champaign *Challenges in Modeling and Simulation of cell-scale systems*
11:10 am	*Q&A*
11:20 am	Break
Session Ib	**Tamar Schlick, NYU, Chair**
11:45 am	Yuji Sugita, RIKEN *Multi-scale molecular dynamics simulations of liquid-liquid phase separation and macromolecular crowding effects*
12:10 pm	*Q&A*
12:20 pm	Jeremy Smith, Oak Ridge National Laboratory/University of Tennessee, Knoxville *Molecular Simulation in the Circular Bioeconomy*
12:45 pm	*Q&A*
12:55 pm	Lunch and Poster Session *Rooms 905-907*
Session IIa	**Rommie Amaro, UC San Diego, Chair**
2:15 pm	Cecilia Clementi, Free University of Berlin *Understanding protein dynamics by combining simulation, experimental data, and machine learning*
2:40 pm	*Q&A*
2:50 pm	Pilar Cossio, Flatiron Institute *Exploring conformational landscapes with molecular simulations and single-particle cryo-EM*
3:15 pm	*Q&A*
3:25 pm	Break
Session IIb	**Rommie Amaro, UC San Diego, Chair**
3:50 pm	Jodi Hadden-Perilla, University of Delaware *AMBERff at Scale: Multimillion-Atom Simulations with AMBER Force Fields in NAMD*

4:00 pm	*Q&A*
4:02 pm 4:12 pm	Glen Hocky, New York University *Good rates from bad coordinates: the exponential average time-dependent rate method (EATR)* *Q&A*
4:14 pm 4:24 pm	Shuting Yan, New York University *Multiple transition pathways between two pseudoknots of the SARS-CoV-2 frameshift element shed insight on viral mechanism* *Q&A*
4:26 pm 4:36 pm	Konstantin Roeder, King's College London *Investigation of structural heterogeneity in RNA through energy landscape explorations* *Q&A*
4:38 pm	Break
Session IIc	**Tamar Schlick, NYU, Chair**
4:45 pm 5:10 pm	David Shaw, DE Shaw Research *Biomolecular Simulation in our Lab: Progress, Problems and Prospects* *Q&A*
5:20 pm	Adjourn



Monday, May 6

Speaker Bios

J. Andrew McCammon, University of California San Diego

J. Andrew McCammon is a Distinguished Research Professor of Chemistry and of Pharmacology at UCSD. He has invented theoretical methods for accurately predicting and interpreting molecular recognition, rates of reactions, and other properties of chemical systems. These methods play a growing role in the design of new drugs and other materials. Professor McCammon is the author with Stephen Harvey of "Dynamics of Proteins and Nucleic Acids" (Cambridge University Press), and is author or co-author of nearly 900 publications in theoretical chemistry and biochemistry. More than 50 of his former students have tenured or tenure-track positions at leading universities or research institutes. In the 1980's, he guided the establishment of computer-aided drug discovery in Agouron Pharmaceuticals (now Pfizer's La Jolla Laboratories), contributing to the development of the HIV-1 protease inhibitor, nelfinavir. His group's studies of HIV-1 integrase flexibility subsequently aided discovery of raltegravir by Merck & Co. His awards include the Smithsonian Institution's Information Technology Leadership Award for Breakthrough Computational Science and the American Chemical Society's National Award for Computers in Chemical and Pharmaceutical Research. He is a Fellow of the American Academy of Arts and Sciences and a Member of the US National Academy of Sciences.

Emad Tajkhorshid, University of Illinois Urbana-Champaign

Emad Tajkhorshid directs the NIH Center for Macromolecular Modeling and Bioinformatics and the Computational Structural Biology and Molecular Biophysics Group at the Beckman Institute. He is Hastings Endowed Chair in the Biochemistry Department, as well as holds additional appointments across multiple colleges that include Chemistry, Bioengineering, Pharmacology, Biophysics and Quantitative Biology, Computational Science and Engineering, and the Carle-Illinois College of Medicine at the University of Illinois. His research focuses on developing and applying advanced computational techniques to characterization of biological phenomena, particularly membranes and membrane proteins, with the aim of achieving the most detailed microscopic view of structural and dynamical bases underlying biological function. Major areas of his extensive research portfolio, which have enjoyed continuous support from multiple federal funding agencies (NIH, NSF, DOE, DOD) over many years, include mechanistic studies of membrane transport proteins, principles of energy transduction and coupling in bioenergetic proteins, and lipid modulation of protein function, e.g., in signaling proteins associated with the cellular membrane. Dr. Tajkhorshid has authored over 200 research articles (H-index 60) with over 20,000 citations in such high-profile journals as *Nature, Science, Cell, eLife,* and *PNAS*. He has delivered nearly 150 invited lectures at international meetings, universities, and research institutes. He has served on the Editorial Boards of multiple major journals, including *Biophysical Journal, Journal of Biological Chemistry,* and *PLoS Computational Biology,* and *Biochemical and Biophysical Research Communication.*

Yuji Sugita, RIKEN

Yuji Sugita is Chief Scientist, Theoretical Molecular Science Laboratory, RIKEN Cluster for Pioneering Research. He is author of over 300 publications in the areas of computational biophysics, protein dynamics and molecular dynamics. His professional associations include The Physical Society of Japan, The Biophysical Society of Japan, The Molecular Simulation Society of Japan, Protein Science Society of Japan, BioSuperComputing Research Community, Biophysical Society(US), and American Chemical Society(US). He is the recipient of the Young Scientist Award of the Physical Society of Japan (Ryoiki 12), the Young Scientist Award of the Molecular Simulation Society of Japan, and the Morino Award for Molecular Science.

Jeremy Smith, Oak Ridge National Laboratory/University of Tennessee, Knoxville

Prof. Jeremy C. Smith has led research groups in France, Germany and the United States. After education at Leeds and London University in 1985 he became a postdoctoral fellow and lecturer with Nobel Laureate Martin Karplus at Harvard University. In 1989 he established a biomolecular simulation group at the Commissariat a l'Energie Atomique in Saclay, near Paris. In 1998 he became Chair of Computational Molecular Biophysics at the University of Heidelberg, and in 2006 became the first University of Tennessee/Oak Ridge National Laboratory Governor's Chair and also Founding Director of the ORNL Center for Molecular Biophysics, which currently encompasses seven research groups. In 2008 he was named Honorary Professor of the University of Heidelberg. He received the ORNL Director's Award for Individual Achievement in

2017. Smith's research interests include the high-performance computer simulation of biological macromolecules, supercomputing, bioenergy, environmental biogeochemistry, drug and vaccine design and biological neutron scattering. He has published over 400 peer-reviewed scientific articles.

Cecilia Clementi, Free University of Berlin

Cecilia Clementi is Einstein Professor of Physics at Freie Universität (FU) Berlin, Germany. She joined the faculty of FU in June 2020 after 19 years as a Professor of Chemistry at Rice University in Houston, Texas. She obtained her Ph.D. in Physics at SISSA and was a postdoctoral fellow at the University of California, San Diego, where she was part of the La Jolla Interfaces in Science program. Her research focuses on the development and application of methods for the modeling of complex biophysical processes, by means of molecular dynamics, statistical mechanics, coarse-grained models, experimental data, and machine learning. Professor Clementi's research has been recognized by a National Science Foundation CAREER Award (2004), and the Robert A. Welch Foundation Norman Hackerman Award in Chemical Research (2009). Since 2016 she is also a co-Director of the National Science Foundation Molecular Sciences Software Institute.

Pilar Cossio, Flatiron Institute

Pilar Cossio is Research Scientist and Project Leader for Structural and Molecular Biophysics (SMB) in the Center for Computational Mathematics at the Flatiron Institute. Dr.. Cossio holds a Ph.D. in Physics and Chemistry of Biological Systems from the International School for Advanced Studies (SISSA) in Italy and a B.S. in Physics from the University of Antioquia. She was Max Planck Tandem Group Leader associated with the University of Antioquia (Colombia) and the Max Planck Institute of Biophysics (Germany). She also has held postdoctoral positions at the National Institute of Health (NIH, USA) and the Max Planck Institute of Biophysics. Dr. Cossio focuses on the development of mathematical and computational methods to characterize proteins' structures and dynamics from cryo-electron microscopy, single-molecule spectroscopy and biomolecular simulations.

Jodi Hadden-Perilla, University of Delaware

Jodi Hadden-Perilla is currently an Assistant Professor with the Department of Chemistry and Biochemistry, University of Delaware. She received her Ph.D. in computational chemistry from the University of Georgia, and carried out Postdoctoral Training with the Beckman Institute, University of Illinois at Urbana-Champaign. Her research group uses molecular dynamics simulations to study biological machines, including viruses, and molecular motors.

Glen Hocky, New York University

Glen Hocky is an Assistant Professor in the Department of Chemistry at New York University, and Simons Center for Computational Physical Chemistry. His research interests lie at the intersection between chemistry, physics, biology, and materials science and broadly involve using (and developing new) techniques from statistical mechanics and computational modeling to better understand how molecular interactions give rise to large scale collective phenomena.

Shuting Yan, New York University

Shuting Yan is a postdoctoral researcher in the Schlick Group at NYU where she works on molecular dynamics simulations of RNA viral frameshifting, and RNA structural transitions using enhanced sampling methods.

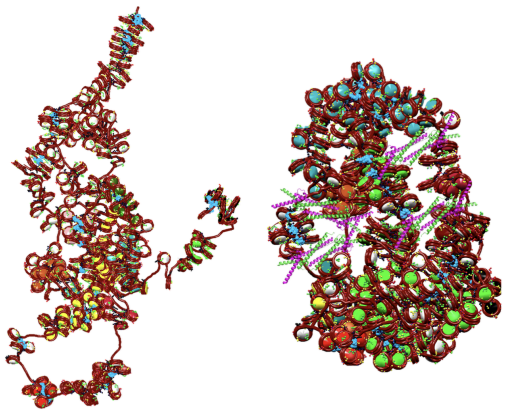
Konstantin Roeder, King's College London

Konstatin Roeder is a Lecturer at the Randall Centre for Cell & Molecular Biophysics at King's College London. His current research interests lie in the development of new methods to explore energy landscapes more efficiently for large biomolecules and in improving the HiRE coarse-grained force field. His research combines computational methods (energy landscape explorations, global optimisation techniques and MD simulations) to gain mechanistic insight into biomolecular behavior, providing meaningful feedback to experimental collaborators.

David Shaw, DE Shaw Research

David Shaw is founder and chief scientist of D. E. Shaw Research, LLC, in which capacity he leads an interdisciplinary research group in the field of computational biochemistry and personally engages in hands-on scientific research in that field. He also holds appointments as a Senior Research Fellow at the Center for Computational Biology and Bioinformatics at Columbia University and as an Adjunct Professor of Biochemistry and Molecular Biophysics at

Columbia's medical school. Dr. Shaw received his Ph.D. from Stanford University in 1980 and served on the faculty of the Computer Science Department at Columbia University until 1986, when he left to pursue the emerging field of computational finance. He initiated his work on computational biochemistry in 2001, and began building the scientific team at D. E. Shaw Research in 2002, and resumed his affiliation with Columbia in 2005. Dr. Shaw was appointed to the President's Council of Advisors on Science and Technology by President Clinton in 1994, and again by President Obama in 2009. He is a two-time winner of the ACM Gordon Bell Prize, and was elected to the American Academy of Arts and Sciences in 2007, to the National Academy of Engineering in 2012, and to the National Academy of Sciences in 2014.



Monday, May 6

Posters
Kimmel Center Rooms 905-907

Author	Poster Title	Author	Poster Title
Alan Ianeselli Yale Univ.	*A novel Discard-and-Restart MD algorithm for the efficient sampling of realistic protein transition states and enhance structure based drug discovery*	Miro Astore Flatiron Institute	*Probing conformational heterogeneity of TRPV1: A comparison of state-of-the-art methods in cryo-EM*
Alexander Bryer Univ. of Delaware	*Human factors modulate the HIV-1 capsid mechanoelastic properties during nuclear import.*	Mohamed Shehata UCSD	*Navigating Protein Design with Confidence: Leveraging Alchemical Free Energy Calculations*
Arjun Singh Rutgers Univ., New Brunswick	*Proteins in Phase: Unveiling the Role of IDPs and Structured Proteins in Biomolecular Condensates*	Myongin Oh Weill Cornell Medicine	*Deciphering the molecular mechanisms of STRA6-mediated retinol transport*
Atanu Acharya Syracuse Univ.	*Building Cheaper Computational Tools to Model Electron Transfer Processes in Biochemistry*	Rutika Patel CUNY Grad Ctr.	*Conformational dynamics of Histone H2B tails using molecular dynamics simulation and Markov state model*
Charlotte Infante NYU	*Unifying pKa and Protonation Prediction with T5Chem-pKa*	Sheeba Malik UT/ORNL	*Decoding Anomalous Diffusion in Frequency Space: Insights into Bilayer Phase Transitions*

Christina Vilchez NC State	*Molecular Modeling of Self-assembly of Nucleic Acid NanoParticles (NANPs)*	Md. Raihan Uddin CUNY	*Using Monte Carlo Microstates to Follow Proton Transport in Complex I*
Dariia Yehorova Georgia Tech.	*Key Interaction Networks (KIN): Unveiling Evolutionarily Conserved Interactions in Beta-Lactamases*	Shintaroh Kubo Univ. of Tokyo	*Investigating Rotational Symmetry Discrepancies between FO and F1 in FOF1 ATPase: A Coarse-Grained MD Simulation Approach*
Eric Chen NYU	*Conformational Selection for Allosteric Docking: Case Study with CDK2*	Song Xia NYU	*Normalized Protein-Ligand Distance Likelihood Score Incorporating Explicit Metal Ions and Ligand Conformation Stability*
Federica Maschietto NYU	*Mapping Allosteric Signals to Manipulate Catalytic Activity*	Subarna Sasmal NYU	*Quantifying Unbiased Conformational Ensembles from Biased Simulations Using ShapeGMM*
Flavia Maria Galeazzi Brown Univ.	*Rapid prediction of protein tyrosine kinase conformational ensembles by combining machine learning predictions with enhanced sampling simulations*	Stephanie Portillo NYU	*Implicit Modeling of Protein Binding to Chromatin Fibers*
Gabriel Monteiro da Silva Brown Univ.	*Accelerating Convergence in Enhanced Sampling Simulations by Predicting Protein Conformational Ensembles*	Vinicius Contessoto Rice Univ.	*Interphase chromosomes of the Aedes aegypti mosquito are liquid crystalline and can sense mechanical cues*
Hemani Chhabra UIUC	*Strand stories - Understanding ssDNA dynamics using all-atom MD simulations guided via high throughput FRET.*	Yan Yu ORNL	*Enhanced biomass pellet properties upon deep eutectic solvent pretreatment and their molecular origins*
Julie Gardella NYU	*Estimating the transplacental transfer of plastic production chemicals using machine learning and in vitro assays with human trophoblast cells to understand toxicity*	Yang Wang Boston College	*Interplay of steric and diffuse ion effects regulates the final stages of aminoacyl-tRNA accommodation*
Kuntal Ghosh Univ. of Chicago	*Embedding quantum mechanics and neural network based force fields into a coarse-grained environment*	Yeonji Ji CUNY Grad. Ctr.	*Solvation Thermodynamics Barriers to Binding Site Formation*
Lauren Intravaia Univ. of Massachusetts	*Elucidating complex mechanisms of HIV-1 protease inhibition and resistance with molecular dynamics and machine learning*	Yudan Shi UT Knoxville	*A Comparative Analysis of TCR Structure Prediction Tools*
Lorenzo Casalino UCSD	*Harnessing molecular simulations to design stabilized SARS-CoV-2 S2 antigens*	Zhuoran Long Yale Univ.	*Dynamic Structures and Functional Roles of Water in Photosystem II Water Channels Investigated with Molecular Dynamics*
M. Margarida Rosa Weill Cornell Medicine	*Automating Collective Variable Discovery from Molecular Dynamics Simulations using Machine Learning'*	Zhuoyi Liu Yale Univ.	*The minimum and optimal restraints in FRET-assisted protein structural modeling*
		Zilong Li NYU	*Hi-BDiSCO: Folding 3D Mesoscale Genome Structures from Hi-C Data using Brownian Dynamics*

Tuesday, May 7

Program
Kimmel Center, Shorin 802

Keynote Talk: 25 min + 10 min Q&A
Short Talk: 10 min + 2 min Q&A

9:30 am	Continental Breakfast
Session IIIa	**Tamar Schlick, NYU, Chair**
10:00 am	Modesto Orozco, IRB Barcelona *Multiscale simulation of nucleic acids*
10:25 am	*Q&A*
10:35 am	José Onuchic, Rice University *Unraveling Chromatin Architecture and Dynamics Through Physical Modeling and Large-Scale Simulations*
11:00 am	*Q&A*
11:10 am	Break
Session IIIb	**Jeremy Smith, ORNL/UT, Chair**
11:30 am	Jessica Swanson, University of Utah *Challenges in multiscale kinetic modeling: Capturing the roles of kinetic selection and electrochemically-driven charge transport*
11:40 am	*Q&A*
11:42 am	Ivan Coluzza, Rice University *The Role of Charges and Solvent in Protein Folding and Aggregation: A Computational Insight*
11:52 am	*Q&A*
11:54 am	Rajitha Tatikonda, UT/ORNL *TCR-H: Machine Learning Prediction of T-cell Receptor Epitope Binding on Unseen Datasets*
12:04 pm	*Q&A*
12:06 pm	Daniele Di Marino, Polytechnic University of Marche *Structural basis of dimerization of chemokine receptors CCR5 and CXCR4*
12:16 pm	*Q&A*
12:18 pm	Break
Session IIIc	**Rommie Amaro, UCSD, Chair**
12:25 pm	Syma Khalid, University of Oxford *Large scale MD simulations of bacterial membranes*
12:50 pm	*Q&A*
1:00 pm	Adjourn

Tuesday, May 7

Speaker Bios

Modesto Orozco, IRB Barcelona

Modesto Orozco is Professor of Biochemistry and Molecular Biology in the Departament de Bioquímica, Universitat de Barcelona, Director Molecular Modelling and Bioinformatics Unit, IRB Barcelona, Director of the Life Sciences Department of the Barcelona Supercomputing Center, and Integrative Research Node coordinator IRB Barcelona. He is Member of the Editorial board of: Journal of Computational Chemistry, Journal of Chemical Theory and Computation, Phys.Chem.Chem.Phys., J.Mol.Recog., J. Mol.Graphics and Modeling, Nucleic Acids Res., and Chem. Professor Orozco's research activity is focused on the theoretical study of biological systems and is reflected in close to 500 papers published in international peer-reviewed journals of the highest impact. His publications have collected more than 35000 citations with an h-index of 93, the highest for a computational chemist in Spain. Among other awards, in 1997 he received the "Diaz de Santos" National Award for young scientist, the Distinción Investigadora de la Generalitat de Catalunya (Annual award of Science of the Catalan Science Ministry) in 2000, the FEBS Anniversary Prize of the Gesellschaft für Biochemie und Molekularbiologie in 2001, the Fundación Marcelino Botín fellowship (2007), the Brucker award for research in biophysics (2010), as well as the ICREA Academy award for excellence in research and the Advanced Grant of the European Research Council. Professor Orozco is founder and president of Nostrum Biodiscovery.

José Onuchic, Rice University

José Onuchic is Harry C. and Olga K. Wiess Chair of Physics, and Professor of Chemistry and BioSciences at Rice University. He has led the biological physics community to devise an integrated picture of a variety of model biochemical and biological systems. His research has expanded across the scales of molecular-level interactions to cellular systems and multicellular structures. At Rice he has moved towards medical applications focusing on cancer. In protein folding, he introduced the concept of protein folding funnels. Convergent kinetic pathways, or folding funnels, guide folding to a unique, stable, native conformation. Energy landscape theory and the funnel concept provide the theoretical framework needed to pose and to address the questions of protein folding and function mechanisms. He also works on the theory of chemical reactions in condensed matter with emphasis on biological electron transfer. He is also interested in stochastic effects in gene networks with connections to bacteria decision-making and cancer. Currently his group is also focusing on chromatin folding and function. He is a Fellow of the American Physical Society, the American Academy of Arts and Sciences, and the Biophysical Society. He is a member of the U.S. National Academy of Sciences, the Brazilian Academy of Sciences, and the Pontifical Academy of Sciences.

Jessica Swanson, University of Utah

Jessica Swanson is a theoretical biophysical chemist in the Henry Eyring Center for Theoretical Chemistry at the University of Utah. Her research has long been focused on the development and use of biophysical simulation methods to characterize the fundamental mechanisms and driving forces behind biomolecular processes, with foci ranging from membrane permeation, targeting, and transport to lasso peptide folding.

Ivan Coluzza, Rice University

Ivan Coluzza is an Ikerbasque Professor, currently serving as a Visiting Professor at Rice University. His research focuses on developing nanomaterials and polymers that mimic biological systems, using advanced computational tools to innovate in medical and technological applications.

Rajitha Tatikonda, UT/ORNL

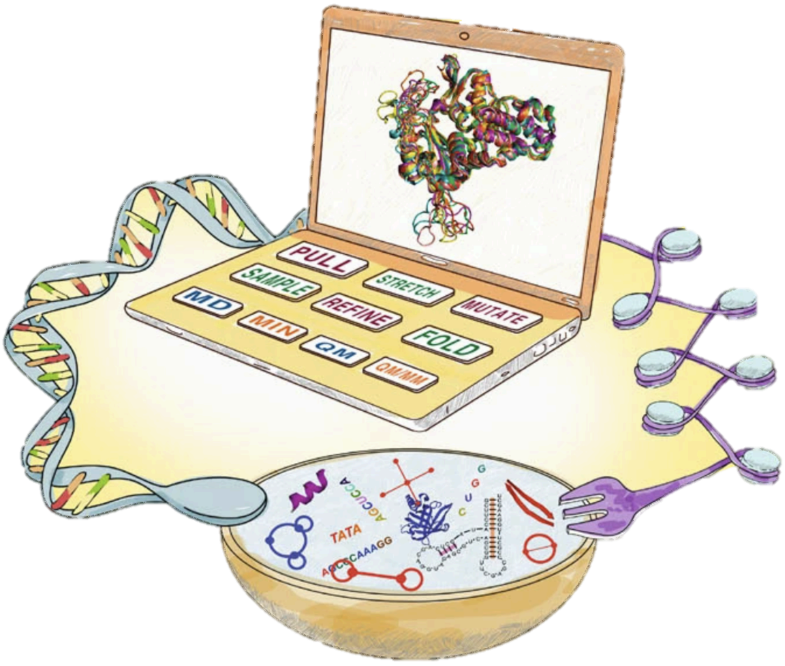
Rajitha Tatikonda is a postdoctoral research associate at the University of Tennessee, Knoxville and UT/ORNL Center for Molecular Biophysics working with Jeremy C Smith. Rajitha's research interests include computational modeling, simulation and machine learning.

Daniele Di Marino, Polytechnic University of Marche

Daniele Di Marino's research interests lie predominantly in computational biophysics, drug design, and bioinformatics, complemented by substantial experience in molecular biology, integrating computational data from enhanced sampling simulations with experimental findings.

Syma Khalid, University of Oxford

Syma Khalid is Professor of Computational Microbiology at the University of Oxford. The main theme in her research is the use of computational techniques to explore the structure-function relationships of a range of microbial membranes/cell envelopes, with a particular focus on Gram-negative bacteria. She is particularly interested in developing computational models that closely mimic *in vivo* systems, in an approach that differs from traditional reductionist approaches often employed within biomolecular simulations. Professor Khalid is the current chair of HECBioSim. She chairs the Technical Advisory Panel of the Artificial Intelligence and Informatics theme of the Rosalind Franklin Institute. She was awarded the Suffrage Science award for engineering and physical sciences in 2021.



Wednesday, May 8

Program
Kimmel Center, Shorin 802

Keynote Talk: 25 min + 10 min Q&A
Short Talk: 10 min + 2 min Q&A

9:00 am	Continental Breakfast
Session IV	**Karissa Sanbonmatsu, LANL, Chair**
9:30 am	Abhishek Singharoy, Arizona State University
	Path integral approaches to study molecular complexity in Latent spaces
9:55 am	*Q&A*
10:05 am	Adrian Mulholland, University of Bristol
	Dynamical-Nonequilibrium Molecular Dynamics Simulations for Enzyme Design, Evolution and Drug Resistance
10:30 am	*Q&A*
10:40 am	Break
11:00 am	David S. Cerutti, Psivant Therapeutics
	Scaling Small Problems to Modern GPUs in the STORMM Code Base
11:10 am	*Q&A*
11:12 am	Yinghao Wu, Albert Einstein College of Medicine
	Understanding how tumor necrosis factor activates the signaling of its different receptors through multiscale simulations
11:22 am	*Q&A*
11:24 am	Tomek Wlodarski, Inst. of Biochem and Biophys, PAS
	Co-translational protein folding in the light of ribosome evolution
11:34 am	*Q&A*
11:36 am	Rongmei Judy Wei, City University of New York
	Electron Transfer Directionality in Type II Photosynthetic Reaction Centers
11:46 am	*Q&A*
11:48 am	Break
12:10 pm	Martin Vögele, Schrödinger, Inc.
	Is the Functional Response of a Receptor Determined by the Thermodynamics of Ligand Binding?
12:20 am	*Q&A*
12:22 pm	Gehan Ranepura, City College of New York
	Inhomogeneous Broadening of Antenna Protein Chlorophyll Site Energies due to Side Chain Conformational and Protonation States determined by Monte Carlo Microstate Analysis
12:32 pm	*Q&A*
12:34 pm	Pinchen Xie, Princeton University
	Dynamically consistent coarse-graining with multi-dimensional generalized Langevin equation
12:44 pm	*Q&A*
12:46 pm	Adjourn

Wednesday, May 8

Speaker Bios

Abhishek Singharoy, Arizona State University

Abhishek Singharoy is an assistant professor in the School of Molecular Sciences at Arizona State University. His research is at the confluence of statistical mechanics, molecular biology, hybrid modeling and large-scale computer simulations. The unified theme of Singharoy laboratory's research is to combine rigorous statistical mechanical methodologies with state-of-the-art computational approaches for capturing cell-scale biological responses with atomic precision. Many of the high-throughput computations essential for approaching this grand challenge are pioneered in the group's past and ongoing work on molecular dynamics, free energy and kinetic modeling methods.

Adrian Mulholland, University of Bristol

Adrian Mulhollad is a Professor of Chemistry, University of Bristol, UK. Following his first degree at Bristol, he worked in a wine merchant and for ICI Pharmaceuticals before doctoral studies with Graham Richards (Oxford) and postdoctoral work with Martin Karplus (Harvard). His research focuses on mechanisms of enzyme catalysis, multiscale modeling, biomolecular dynamics and function. He develops and applies biomolecular simulation methods to problems in antimicrobial resistance, drug metabolism, biocatalysis and enzyme design and evolution. He has published over 250 papers, attracting over 10,000 citations. He has held fellowships from EPRSC and the Wellcome Trust and is an ERC Advanced Grant holder. He established and led CCPBioSim and HECBioSim, and has served as chair of these consortia and of the Molecular Graphics and Modelling Society. He was awarded the 2020 John Meurig Thomas Medal 'for outstanding and innovative work in catalytic science'.

David S. Cerutti, Psivant Therapeutics

David Cerutti has worked in molecular simulations for more than twenty years and developed a number of code bases. His most recent work builds bridges between conformer generation, docking, and molecular dynamics for free energy calculations. As of Oct 26, 2023 STORMM holds over 252,000 lines of original C++ and CUDA code, with its own file parsing, user input design, unit testing, and numerical methods. Psivant's objective is to develop a multi-functional simulation engine with the highest possible utilization of HPC resources. The code base will be released in open-source format to encourage contributions, improvements, and open science within the computational chemistry community.

Yinghao Wu, Albert Einstein College of Medicine

Yinghao Wu is an associate professor at Albert Einstein College of Medicine, Department of Systems and Computational Biology, currently focused on developing multiscale simulation methods to study protein complex assembly as well as understanding the mechanisms of membrane receptor spatial organizations and how these spatial organizations regulate downstream signaling pathways.

Tomek Wlodarski, Inst. of Biochem and Biophys, PAS

Tomek Wlodarski is a computational biophysicist who recently joined the Department of Bioinformatics at the Institute of Biochemistry and Biophysics Polish Academy of Sciences in Warsaw, Poland. His primary scientific focus is to understand how proteins fold and assemble in the cellular environment and how evolution has shaped these processes. His approach involves various computational methods, including multiscale MD simulations and bioinformatics, and takes advantage of available experimental data.

Rongmei Judy Wei, City University of New York

Rongmei Judy Wei is a PhD candidate in computational chemistry at CUNY. Her work in protein modeling focuses on exploring the electrostatic potentials on the electron transfer path, aiming to activate the dormant electron transport pathway, thereby creating dual active electron transfer branches. This amplifies the electron transfer efficiency and increases the energy conversion rate by converting solar energy to chemical reaction energy.

Martin Vögele, Schrödinger, Inc.

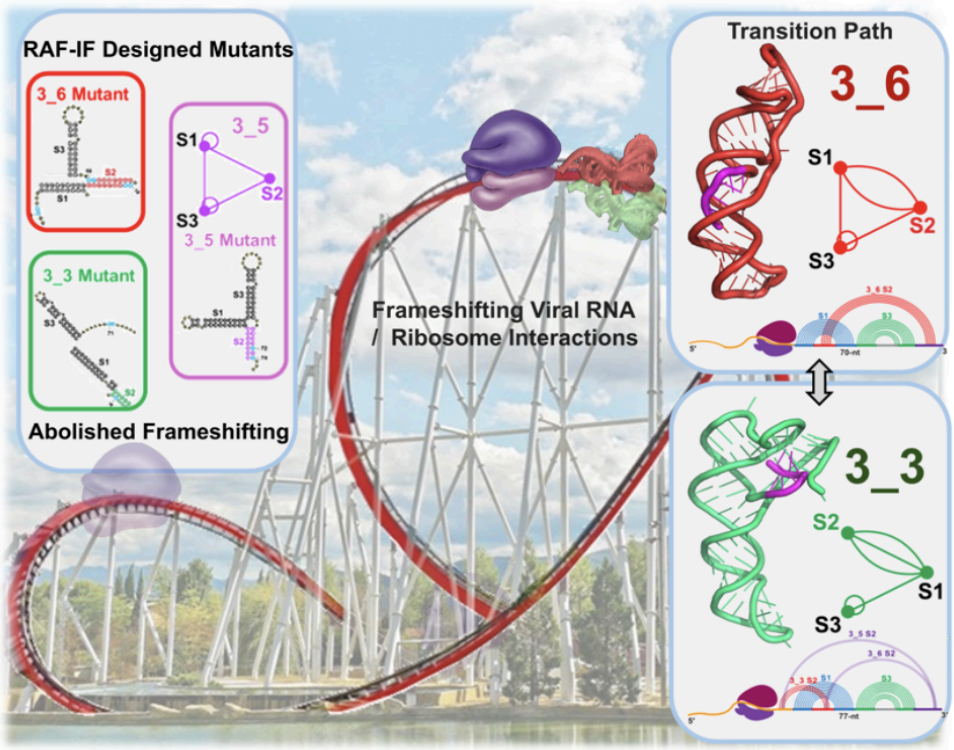
Martin Vögele is a senior scientist at Schrödinger specializing in membrane protein simulations and free energy calculations. His scientific career has been dedicated to pushing the boundaries of molecular simulations, focusing on the unique challenges presented by membranes and membrane proteins. He has spearheaded numerous projects which have advanced the understanding and capabilities in this field, from lipid diffusion in membranes over the pore formation process of membrane-active toxins to the intricate mechanisms of signaling via G protein–coupled receptors.

Gehan Ranepura, City College of New York

Gehan Ranepura is a PhD candidate in physics at CUNY. He is currently investigating the use of a Monte Carlo microstate analysis coupled with pigment chlorophyll site energies calculated using the charge density coupling method to characterize protein to pigment network correlations. By developing and utilizing python based scripts for data analysis and calculations, he aims to differentiate a network of the residues responsible for the bioenergetics of protein function.

Pinchen Xie, Princeton University

Pinchen Xie is a graduate student in the Program of Applied and Computational Mathematics of Princeton University who will join Lawrence Berkeley Lab as an Alvarez fellow in Oct. 2024. Pinchen's interest is developing computational methods for multi-scale biomolecular modeling.



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