

Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, Sixteenth Round

Committee

Chung Wong

Chair

Chung Wong is a Professor in the Department of Chemistry and Biochemistry at the University of Missouri–St. Louis. He previously held research positions at several institutions and has been active in the field of computational biosciences for several decades. His research centers on the development and application of computational methods to investigate biomolecular structure, dynamics, and function, with an emphasis on drug discovery through the integration of molecular simulations, informatics, and machine learning.

Dr. Wong has extensive experience in molecular dynamics simulations of biomolecules, having utilized a range of advanced computing architectures since the 1980s, including systems at the National Center for Supercomputing Applications, the John von Neumann Center, the Houston Area Research Center, the Pittsburgh Supercomputing Center, the San Diego Supercomputer Center, and the Extreme Science and Engineering Discovery Environment (XSEDE) supported by the National Science Foundation.

He earned his Ph.D. in Chemistry from the University of Chicago and completed postdoctoral research at the University of Houston under Professor J. Andrew McCammon.

Ravinder Abrol

Member

Ravinder (“Ravi”) Abrol is a Professor of Chemistry and Biochemistry at California State University, Northridge. His research focuses on developing and applying enhanced conformational sampling methods based on molecular dynamics to study the structure, dynamics, and biochemical interactions of G protein–coupled receptors (GPCRs) with their intracellular transducers, such as G proteins and arrestins. Dr. Abrol’s work seeks to elucidate how GPCR conformational ensembles control signaling and physiology and to apply this knowledge toward the rational design of drugs targeting GPCR signaling pathways. His research contributes to a deeper understanding of these complex membrane proteins as dynamic biophysical machines central to cellular communication. Dr. Abrol has served on numerous National Institutes of Health (NIH) study sections and has participated in multiple review panels for allocation of supercomputing time on Anton. He earned a B.Sc. (Honours) in Chemistry from the University of Delhi, an M.Sc. in Chemistry from the Indian Institute of Technology Kanpur, and a Ph.D. in Chemistry from the California Institute of Technology.

Nilesh Banavali

Member

Dr. Banavali is a Research Scientist in the Division of Translational Medicine at the Wadsworth Center, New York State Department of Health. He has extensive expertise in molecular mechanics force field development, free energy determination, enhanced sampling methods, and structure prediction, with additional specialization in modeling biochemical reaction mechanisms and structural analysis using single-particle cryo-electron microscopy. His research has contributed to significant advances in computational biophysics, including the determination of the free energy landscape of A-form to B-form conversion in DNA, identification of the B-form in RNA, elucidation of the dynamic mechanism underlying DNA insertion-deletion mutations, and discovery of the molecular basis of allosteric regulation in protein tyrosine kinases. His work has also provided insights into the evolutionary increase in protein content of eukaryotic ribosomes.

Dr. Banavali earned a B.S. in Pharmaceutical Sciences from the University of Mumbai and a Ph.D. in Pharmaceutical Sciences from the University of Maryland, Baltimore. He completed postdoctoral research in molecular dynamics method development at Weill Medical College of Cornell University and the University of Chicago.

James Briggs

Member

James Briggs, Ph.D., is the Associate Provost for Faculty Development and Faculty Affairs and a Professor in the Department of Biology and Biochemistry at the University of Houston. He previously served as Chair of the department and has extensive experience in faculty leadership, research administration, and mentoring.

Dr. Briggs's research focuses on computational studies of protein structure and function, inhibitor design, and the prediction of inhibitor resistance pathways, as well as the development of novel computational methods to advance these areas. His work spans two major themes: computer-aided inhibitor discovery and computational biophysics. His target systems include Rho kinase 1 (heart disease), PTEN and BCL2 (cancer), PTEN/5HTC2C (addiction control), and pathways related to gluconeogenesis and glucose uptake. In computational biophysics, his studies address cholera toxin, biofilm regulation, RNA structure prediction, protein electrostatics, and pKa prediction.

Dr. Briggs received his Ph.D. in Theoretical Organic Chemistry from Purdue University. He has served multiple times on National Academies' Molecular Dynamics Review Committees, including as Chair for the 2019 evaluation cycle.

Jianhan Chen

Member

Jianhan Chen, Ph.D., is a Professor in the Department of Chemistry at the University of Massachusetts Amherst. He leads a research program dedicated to the development of theoretical and computational methods to advance understanding of fundamental biophysical, biochemical, and biomedical processes.

Dr. Chen's work addresses key challenges in biomolecular science, including the roles of intrinsically disordered proteins in health and disease, mechanisms of protein amyloid formation in neurodegenerative disorders, the design of self-assembling peptide vesicles for drug delivery, and the activation and regulation of transmembrane ion channel proteins. His research integrates physics-based modeling, statistical mechanics, and molecular simulation to provide insights into complex biological phenomena.

Dr. Chen has received several distinctions for his contributions to computational biophysics, including the NSF CAREER Award (2010), the ACS Outstanding Junior Faculty Award (2011), and the Outstanding Research Award from the UMass College of Natural Sciences (2022). He earned his Ph.D. in Chemical and Material Physics from the University of California, Irvine, in 2002.

Ryan Cheng

Member

Ryan Cheng, Ph.D., is an Assistant Professor in the Department of Chemistry at the University of Kentucky, where he joined the faculty in 2022. Before his appointment, he conducted postdoctoral research at the Center for Theoretical Biological Physics at Rice University.

Dr. Cheng's research integrates computer simulations, biopolymer theory, statistical mechanics, and machine learning to investigate the physical principles underlying genome organization and transcriptional regulation. His group seeks to uncover how genetic material is spatially organized within eukaryotic cell nuclei and how biomolecular interactions govern this organization to influence gene expression, genome maintenance, and cellular function. By combining computational modeling with theoretical approaches, his work aims to bridge molecular-scale processes with emergent biological behavior.

Dr. Cheng's interdisciplinary research contributes to a deeper understanding of the complex interplay between genome architecture and function, offering insights relevant to molecular biology, biophysics, and computational chemistry.

Brian Dominy

Member

Brian Dominy, Ph.D., is an Associate Professor of Chemistry at Clemson University, where he has been a faculty member since 2005. He currently serves as Associate Dean in the Division of Undergraduate Learning, supporting student success through academic policy, curricular oversight, and institutional process improvement. His previous administrative roles include Director of Undergraduate Studies in the Department of Chemistry (2011–2016), Interim Associate Dean for Academic Affairs in the College of Science (2016–2018), and Associate Dean for Academic Policy and Program Effectiveness in the Graduate School (2018–2024).

As a computational biophysical chemist, Dr. Dominy leads a research program that investigates the physicochemical forces underlying biomolecular function and evolution. His work combines molecular simulations and theoretical approaches to better understand how biological macromolecules achieve structural stability and catalytic efficiency.

Dr. Dominy earned his Ph.D. in Chemistry from The Scripps Research Institute in 2001 and was a Ruth L. Kirschstein Postdoctoral Fellow at Harvard University before joining Clemson. He has previously served on multiple Molecular Dynamics Review Committees convened by the National Academies, and chaired the committee in 2024.

David Eike

Member

David Eike, Ph.D., is a Director Principal Scientist at the Procter & Gamble Company, where he leads efforts in applying physics- and data-based modeling to the design and optimization of consumer goods and personal care products. His work integrates computational chemistry, materials science, and engineering to understand and predict complex formulation behaviors that drive product performance.

Dr. Eike has extensive experience using both atomistic and coarse-grained molecular dynamics simulations to study the self-assembly and multiscale behavior of colloidal materials such as surfactants and polymers. His research has advanced the ability to model and design soft-matter systems with improved functional properties.

He has received supercomputing allocations through the Extreme Science and Engineering Discovery Environment (XSEDE) Industry Challenge and the Oak Ridge Leadership Computing Facility, supporting large-scale simulations for industrial applications. Dr. Eike earned his Ph.D. in Chemical Engineering from the University of Notre Dame.

James C. Gumbart

Member

James (JC) Gumbart, Ph.D., is the Dunn Family Professor of Physics at the Georgia Institute of Technology. He has over two decades of experience in molecular dynamics (MD) simulations of biomolecular systems, with particular expertise in membrane proteins. His research combines physics-based modeling and large-scale computation to elucidate the structural and energetic principles underlying biomolecular function and dynamics.

Dr. Gumbart's expertise encompasses force-field parameterization, free-energy calculations, and the development and application of advanced MD simulation methodologies. His work has contributed to improving the accuracy, scalability, and interpretability of computational models for complex biological systems.

He earned his Ph.D. in Physics from the University of Illinois at Urbana-Champaign under the mentorship of Klaus Schulten and completed postdoctoral research as a Director's Postdoctoral Fellow at Argonne National Laboratory with Benoît Roux. Dr. Gumbart has utilized the first Anton supercomputer at the Pittsburgh Supercomputing Center and has served as a reviewer for subsequent Anton proposal cycles since 2017.

Ellinor Haglund

Member

Ellinor Haglund, Ph.D., is an Associate Professor in the Department of Chemistry at the University of Hawai'i at Manoa. Her research focuses on the folding, structure, and function of proteins with complex topologies, integrating computational and experimental approaches to elucidate fundamental principles of protein behavior.

Dr. Haglund's laboratory combines Molecular Dynamics (MD) simulations with in vitro and in vivo biological assays to investigate how topologically intricate proteins achieve their native structures and carry out their biological functions. This interdisciplinary work bridges chemistry, biophysics, and molecular biology to provide insight into protein folding mechanisms and their broader biological implications.

In recognition of her research contributions, Dr. Haglund received the National Science Foundation CAREER Award in 2020. She has also served as a member of the Anton Computer Committee since 2020, supporting national efforts to advance computational resources for biomolecular simulation.

Yu-ming M. Huang

Member

Ying Huang is an Assistant Professor in the Department of Physics and Astronomy at Wayne State University. Her research focuses on developing and applying computational and theoretical methods to study biomolecular recognition, protein-ligand binding kinetics, and diffusion processes. Dr. Huang's group integrates molecular dynamics simulations with statistical modeling to uncover the mechanisms governing protein-lipid interactions and enzyme activation processes relevant to human health and disease. She received her Ph.D. in Computational Chemistry from the University of California, Riverside, in 2014, and completed postdoctoral training at the University of California, San Diego, in 2019. Dr. Huang's contributions to computational biophysics have been recognized with several honors, including the Wiley Computers in Chemistry Outstanding Postdoc Award, the Protein Science Best Paper Award, and the NIH R35 MIRA Award. She has served on the ANTON supercomputer review panel and has participated in multiple National Institutes of Health (NIH) review panels.

Andrzej Kloczkowski

Member

Andrzej Kloczkowski, Ph.D., is a Principal Investigator in the Institute for Genomic Medicine at Nationwide Children's Hospital and a Professor of Pediatrics and Biomedical Informatics at The Ohio State University. His research focuses on computational molecular biology and structural bioinformatics, with an emphasis on systems biology, protein structure prediction, and the modeling of biomolecular dynamics and function.

Dr. Kloczkowski's work spans multiple levels of biological organization, integrating genomics, biophysics, and informatics to uncover the principles governing molecular structure and biological regulation. His research has been supported by numerous grants from the National Institutes of Health and the National Science Foundation.

He earned his Ph.D. from the Institute of Physical Chemistry of the Polish Academy of Sciences in Warsaw, Poland, and completed postdoctoral training at Stanford University. Dr. Kloczkowski has also served multiple terms on the National Research Council Committee for the Allocation of Supercomputing Time for the Study of Molecular Dynamics.

Albert Lau

Member

Albert Lau, Ph.D., is a Teaching Professor in the Department of Biophysics at Johns Hopkins University. His research focuses on the structural thermodynamics underlying ligand binding, conformational transitions, and allosteric communication in biological macromolecular machines, with particular emphasis on neurotransmitter receptors. Molecular dynamics simulations are a central tool in his studies, enabling detailed insight into protein function and regulation.

Dr. Lau's work integrates computational and theoretical approaches to reveal the molecular mechanisms that govern macromolecular behavior and inform experimental design. His research has been recognized with Johns Hopkins University's Catalyst and Synergy Awards for outstanding contributions to biophysics.

He earned his Ph.D. in Biophysics from Harvard University and a B.S. in Physics with Highest Honors from the University of Michigan. He completed postdoctoral training in computational and structural biophysics under Prof. Benoît Roux at the University of Chicago and Weill Cornell Medical College.

Xiaorong Liu

Member

Xiaorong Liu, Ph.D., is an Assistant Professor in the Department of Chemistry and Chemical Biology at the University of New Mexico. Prior to her appointment at UNM, she conducted postdoctoral research in the laboratory of Professor Charles L. Brooks III at the University of Michigan.

Dr. Liu's research focuses on the development and application of computational methods to guide the design of small-molecule drugs, biologics, and functional proteins, as well as to investigate the sequence-structure-function relationships in proteins. Her laboratory integrates molecular simulations with theoretical and computational modeling to understand biomolecular mechanisms and inform rational design. She has more than a decade of experience performing molecular dynamics simulations of biomolecules.

Her contributions have been recognized with the William E. McEwen Graduate Fellowship in 2018. Dr. Liu earned her Ph.D. in Chemistry from the University of Massachusetts Amherst in 2019.

Mihaly Mezei

Member

Dr. Mezei is an Associate Professor at the Icahn School of Medicine at Mount Sinai, where he has served since 1991 and has held a part-time appointment since 2017. He previously directed the Molecular Modeling Core at Mount Sinai and, earlier in his career, was Research Associate and later Director of the Molecular Graphics Laboratory at Hunter College, CUNY, following postdoctoral research at New York University.

His research focuses on the development and application of computational methodologies for biological systems, including contributions to Monte Carlo sampling techniques, free-energy simulation methods, and novel approaches for analyzing macromolecular systems. Dr. Mezei has also developed software implementing these methods, which is freely available for academic use. His current work emphasizes molecular dynamics simulations of the thyroid-stimulating hormone receptor, utilizing the Minerva supercomputer at Mount Sinai.

He is a member of the American Chemical Society, Biophysical Society, New York Academy of Sciences, and Sigma Xi. Dr. Mezei earned his University Diploma in Chemistry from Eötvös Loránd University in 1967 and his Ph.D. in 1972, with postdoctoral training at NYU and Hunter College. He has served on the NSF Supercomputer Allocation Committee and on committees awarding time on leadership-class systems.

C. Denise Okafor

Member

Denise Okafor is an Assistant Professor in the Departments of Biochemistry and Molecular Biology and Chemistry at Pennsylvania State University. Her research integrates molecular dynamics simulations with biochemical experiments to elucidate the mechanisms of transcriptional activation in nuclear receptors. Prior to her current position, Dr. Okafor earned an M.S. in Computational Chemistry and a Ph.D. in Biochemistry, both from the Georgia Institute of Technology. Since establishing her laboratory in 2020, she has focused on bridging computational and experimental biophysics to understand the molecular basis of receptor signaling and allosteric regulation. Dr. Okafor is the recipient of several prestigious awards, including the NIH Director's New Innovator Award, the Burroughs Wellcome Fund Career Award at the Scientific Interface (CASI), and the NSF CAREER Award. She has also received the Early Career Award from the Theory and Computation Subgroup of the Biophysical Society and the ACS COMP Cadence/OpenEye Outstanding Junior Faculty Award. Dr. Okafor has previously served on the National Academies of Sciences, Engineering, and Medicine (NASEM) review panel for the Anton supercomputer.

Steven W. Rick

Member

Steven W. Rick is a Professor in the Department of Chemistry at the University of New Orleans. His research applies theoretical and computational chemistry approaches to investigate a broad range of molecular systems, including liquid water, aqueous interfaces, proteins, and polymers. Dr. Rick's work focuses on developing improved molecular models and more efficient computer simulation methods to better understand the fundamental interactions governing chemical behavior in complex systems. Prior to his current position, he completed his postdoctoral research at Columbia University after earning a Ph.D. in Chemistry from the University of California, Berkeley, in 1989, and a B.S. in Chemistry from the University of California, Los Angeles. His contributions have advanced the accuracy and scope of molecular dynamics simulations and their applications in chemical and biochemical research. Dr. Rick has previously served on a molecular dynamics review committee convened by the National Academies of Sciences, Engineering, and Medicine.

Leonor Saiz

Member

Leonor Saiz, Ph.D., is a Professor in the Department of Biomedical Engineering at the University of California, Davis. Her research focuses on the dynamics of biological networks at both the molecular and cellular levels, combining computational and theoretical approaches with experimental data to understand how cellular behavior emerges from the interactions and physical properties of its components.

Dr. Saiz's work seeks to infer detailed molecular properties, such as in vivo DNA mechanics, from observed cellular physiology. Her research aims to trace the effects of molecular perturbations—such as protein mutations or interventions with small molecules or drugs—through different levels of biological organization, from molecular changes to cellular and population-level outcomes, addressing one of the major challenges in modern biomedical science.

She earned her Ph.D. in Physics from the University of Barcelona, Spain. Dr. Saiz has participated in multiple rounds of the National Academies of Sciences, Engineering, and Medicine's Molecular Dynamics Review Committee, contributing her expertise in computational biophysics and systems modeling.

Yuk Sham

Member

Yuk Sham is an Associate Professor at the University of Minnesota Medical School and serves as the Director of Graduate Studies for the Bioinformatics and Computational Biology Graduate Program. His research focuses on developing consistent computational structural models to understand the fundamental forces that govern biomolecular recognition. These models provide a foundation for the discovery and design of novel cardiovascular, antiviral, antibacterial, and anticancer therapeutics. Prof. Sham received his Ph.D. in Computational Chemistry under the mentorship of Professor Arie Warshel, recipient of the 2013 Nobel Prize in Chemistry. As a postdoctoral fellow, he was a member of IBM's BlueGene team that developed the world's fastest supercomputer of its time, recognized with the U.S. National Medal of Technology and Innovation in 2009. Earlier in his career, he served as Lead Scientific Consultant at the Minnesota Supercomputing Institute from 2002 to 2008, specializing in molecular dynamics simulations and drug discovery. He served as a faculty member on the Minnesota Supercomputing Institute High Performance Computing Allocation Committee from 2010 – 2016.

Jeffrey Skolnick

Member

Jeffrey Skolnick, Ph.D., is a Regents' Professor and Director of the Center for the Study of Systems Biology in the School of Biological Sciences at the Georgia Institute of Technology. He holds the Mary and Maisie Gibson Chair in Computational Systems Biology, is a Georgia Research Alliance Eminent Scholar in Computational Systems Biology, and serves as Thrust Lead for Precision Medicine and Drug Discovery in the Institute for Data Engineering and Science (IDEaS). He is also Chief Scientific Officer of the Ovarian Cancer Institute.

Dr. Skolnick's research focuses on computational biology and bioinformatics, with an emphasis on AI-based approaches for predicting disease mode-of-action proteins, drug efficacy and side effects, diagnostic tools for early-stage cancer, and non-Mendelian approaches to precision medicine. His work has applications in aging, cancer, chronic fatigue syndrome, and cancer metabolomics, and he has conducted fundamental research on the possible origins of the biochemistry of life.

He received his Ph.D. in Chemistry from Yale University and completed a postdoctoral fellowship at Bell Laboratories. He has held faculty positions at Louisiana State University, Washington University, and the Scripps Research Institute. Among his honors are the SURA Distinguished Scientist Award, Sigma Xi Sustained Research Award, and an Alfred P. Sloan Research Fellowship. He is a Fellow of the AAAS, the Biophysical Society, and the St. Louis Academy of Science, and has authored over 415 publications with an h-index of 96.

Lela Vukovic

Member

Jeffrey Skolnick, Ph.D., is a Regents' Professor and Director of the Center for the Study of Systems Biology in the School of Biological Sciences at the Georgia Institute of Technology. He holds the Mary and Maisie Gibson Chair in Computational Systems Biology, is a Georgia Research Alliance Eminent Scholar in Computational Systems Biology, and serves as Thrust Lead for Precision Medicine and Drug Discovery in the Institute for Data Engineering and Science (IDEaS). He is also Chief Scientific Officer of the Ovarian Cancer Institute.

Dr. Skolnick's research focuses on computational biology and bioinformatics, with an emphasis on AI-based approaches for predicting disease mode-of-action proteins, drug efficacy and side effects, diagnostic tools for early-stage cancer, and non-Mendelian approaches to precision medicine. His work has applications in aging, cancer, chronic fatigue syndrome, and cancer metabolomics, and he has conducted fundamental research on the possible origins of the biochemistry of life.

He received his Ph.D. in Chemistry from Yale University and completed a postdoctoral fellowship at Bell Laboratories. He has held faculty positions at Louisiana State University, Washington University, and the Scripps Research Institute. Among his honors are the SURA Distinguished Scientist Award, Sigma Xi Sustained Research Award, and an Alfred P. Sloan Research Fellowship. He is a Fellow of the AAAS, the Biophysical Society, and the St. Louis Academy of Science, and has authored over 415 publications with an h-index of 96.