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

Committee

Jeffrey Skolnick

Chair

Jeffrey Skolnick is a Regents' Professor in the School of Biological Sciences at the Georgia Institute of Technology. He is also the Mary and Maisie Gibson Chair in Computational Systems Biology and a Georgia Research Alliance Eminent Scholar in Computational Systems Biology. His current research interests are in computational biology and bioinformatics. He has developed AI-based approaches to predict disease mode of action proteins, drug efficacy and side effects including a focus on non-additive pain relievers, and a non-Mendelian approach to precision medicine. Among his awards are the Southeastern Universities Research Association Distinguished Scientist Award, the Sigma Xi Sustained Research Award, and an Alfred P. Sloan Research Fellowship. He is a Fellow of the American Association for the Advancement of Science, the Biophysical Society, and the St. Louis Academy of Science. Skolnick received a Ph.D. in chemistry from Yale University and was a postdoctoral fellow at Bell Laboratories.

Ravinder Abrol

Member

Ravinder "Ravi" Abrol is an Associate Professor of Chemistry and Biochemistry at California State University, Northridge. His research lab is focused on developing and using enhanced conformational sampling methods based on molecular dynamics (MD) to probe how protein structure, dynamics, and biochemical interactions of G protein-coupled receptors (GPCRs) with their intracellular transducers (like G proteins and arrestins) determine cellular signaling and physiology, as well as, how this knowledge can be used for the rational design of drugs targeting GPCR signaling pathways. GPCRs are integral membrane proteins that are emerging as very complex biophysical machines whose signaling profiles are controlled by their conformational ensembles. He has served on numerous study sections for the National Institutes of Health. Abrol received a B.Sc. (Honours) in Chemistry from the University of Delhi, India, an M.Sc. in Chemistry from the Indian Institute of Technology Kanpur, and a Ph.D. in Chemistry from the California Institute of Technology. He has served on the review panels for previous rounds of proposal evaluation for allocation of supercomputing time for the study of molecular dynamics.

Ioan Andricioaei

Member

Dr. Ioan Andricioaei is Professor of Chemistry at the University of California, Irvine. Prior to UCI, he completed his postdoctoral training at Harvard University and served as Assistant Professor at the University of Michigan, Ann Arbor. Dr. Andricioaei's research explores theoretical and computational topics at the interface between molecular biophysics and physical chemistry, including developing novel theoretical techniques and applying computer and modeling methods to describe biologically important molecular processes. Specific research directions include enhanced sampling in trajectory space, computer simulations of DNA-binding machines, and investigating dynamics-function relationships. He received his PhD in Chemistry from Boston University. He is a previous recipient of an NSF CAREER award, and previously served as a committee member on the 3rd round of proposal evaluations.

Jerome Baudry

Member

Jerome Baudry is the Mrs. Pei-Ling Chan Professor of Biological Sciences at the University of Alabama, Huntsville. Prior to his current position, he worked in the pharmaceutical industry as a Research Scientist, and as an assistant professor at the University of Tennessee (UT), Knoxville and the UT/Oak Ridge National Laboratory Center for Molecular Biophysics as a tenure track Assistant Professor in 2008. Baudry's group develops and applies methods and protocols for computational drug discovery, both on small-molecules and biologicals, within academic, national laboratories, and industrial collaborations. Baudry received a Ph.D. in molecular biophysics with the highest Honors from Sorbonne University, Paris, France and completed postdoctoral training at the University of Illinois Urbana-Champaign.

James Briggs

Member

James Briggs is a Professor in the Biology and Biochemistry Department at the University of Houston. His research focuses on computational studies of protein structure and function, inhibitor design, investigations of possible inhibitor resistance pathways, and development of methods for the above areas. Targets for these studies include those important in the treatment of AIDS, cancer, bacterial infections, and other disease states. In addition, Briggs has worked on inhibitors to aid in biowarfare defense (botulinum neurotoxins, anthrax toxin, cholera toxin). His research is focused in the highly interdisciplinary and collaborative area of computational chemistry/biochemistry. His research falls into two general categories: computer-aided inhibitor design/discovery and computational biophysics. Briggs received a Ph.D. in chemistry from Purdue University. He has served on the review panels for previous rounds of proposal evaluation for allocation of supercomputing time for the study of molecular dynamics, including chairing the 10th round in 2019.

Rose K. Cersonsky

Member

Rose Cersonsky is an assistant professor in the Department of Chemical and Biological Engineering at the University of Wisconsin-Madison. Her research involves developing and applying computational methods including machine learning algorithms for the application of molecular dynamics, including specific expertise in materials interfaces and interactions with macromolecular systems across multiple length scales. In addition to research, Rose has devoted herself to scientific service, leading and coordinating multiple outreach programs and publishing work focused on community engagement and gender equity in peer-reviewed journals. Her service work focuses on using communication as a vehicle for promoting inclusivity in the sciences by fostering relationships between primary, secondary, and higher educational institutions and providing approachable scientific material for non-university audiences. Cersonsky received the Victor K. LaMer Dissertation Award from the American Chemical Society, the Charles G. Overberger Award for Excellence in Research, and the Biointerfaces Institute Student Innovator Award. Cersonsky received a B.S. in materials science and engineering from the University of Connecticut and a Ph.D. in macromolecular science and engineering from the University of Michigan. She was a postdoctoral researcher in the Laboratory of Computational Science and Modeling (COSMO) at École Polytechnique Fédérale de Lausanne (EPFL) in Lausanne, Switzerland.

Thomas E. Cheatham, III

Member

Thomas Cheatham, III is a Professor of Medicinal Chemistry and Director of the Center for High Performance Computing at the University of Utah. His research lab uses and develops molecular dynamics, free energy simulation, and trajectory analysis methodologies in applications aimed at better understanding biomolecular structure, dynamics, and interactions. A strong focus of the lab’s efforts centers on the reliable representation of nucleic acid systems (DNA and RNA) in solution. He currently serves as the acting Chair of the Campus Research Computing Consortium. Cheatham received a B.A. in chemistry and a B.A. in mathematics and computer science from Middlebury College and a Ph.D. in pharmaceutical chemistry from the University of California, San Francisco. He was an NRC postdoctoral fellow at the National Institutes of Health.

Ryan Cheng

Member

Ryan Cheng is currently an Assistant Professor of Chemistry at the University of Kentucky. His research group specializes in theory and simulation of biomolecules, particularly coarse-grained simulations of genome organization. Prior work focused on the loop closure of long disordered polymer chains and the role of internal friction as well as on amino acid co-evolutionary information in the context of bacterial signaling networks. He is a full member of Sigma Xi. Cheng received a B.S. in chemistry from Carnegie Mellon University and a Ph.D. in theoretical chemistry from the University of Texas at Austin.

Brian Dominy

Member

Brian Dominy is an Associate Professor in the Department of Chemistry and Associate Dean of the Graduate School at Clemson University. His research focuses on the development and application of computational models to study the physical chemistry driving biomolecular evolution. Dominy's service responsibilities over the years have focused significantly on the development and assessment of academic programs at the departmental, college, and university levels at Clemson. Dominy served as the interim associate dean of academic affairs for the newly formed College of Science from 2016 to 2018, and since 2018 has served as the associate dean for academic policy and program effectiveness in Clemson University's graduate school. He is the recipient of an NSF CAREER award. Dominy received a B.S. with honors in biological sciences and computer science with a minor in chemistry from Carnegie Mellon University and a Ph.D. in biophysical chemistry from Scripps Research Institute. He was an NIH Ruth L. Kirschstein postdoctoral fellow at Harvard University in the Department of Chemistry and Chemical Biology.

James C. Gumbart

Member

James C. "J.C." Gumbart is a Professor of Physics at the Georgia Institute of Technology. His lab carries out molecular dynamics simulations aimed primarily at understanding the composition, construction, and function of the Gram-negative bacterial cell envelope. Gumbart received a B.S.in physics from Western Illinois University and a PhD in physics from the University of Illinois, Urbana-Champaign. He was a postdoctoral fellow at Argonne National Laboratory. He has served on the review panels for previous rounds of proposal evaluation for allocation of supercomputing time for the study of molecular dynamics.

Jodi A. Hadden-Perilla

Member

Jodi A. Hadden-Perilla is an Assistant Professor in the Department of Chemistry & Biochemistry at the University of Delaware. She holds Affiliated Faculty positions in the University of Delaware's Data Science Institute and Center for Bioinformatics & Computational Biology. Her expertise includes molecular modeling and molecular dynamics simulations, as well as classical force field parameterization and interoperability. She has extensive experience performing and analyzing simulations encompassing millions of atoms to decipher biomolecular structure-function relationships. She has previously been granted allocations on Anton 2, XSEDE/ACCESS, and leadership-class supercomputers. Hadden-Perilla is a Deputy Editor for the Journal of Structural Biology, the social media editor for Current Opinion in Structural Biology and serves on the Advisory Board for the University of Delaware's Center for Data-intensive & Computational Science. Hadden-Perilla received a Ph.D. in computational chemistry from the University of Georgia and completed postdoctoral training in biophysics at the Beckman Institute at the University of Illinois Urbana-Champaign.

Ellinor Haglund

Member

Ellinor Haglund is currently an Assistant Professor in the Department of Chemistry at the University of Hawaii at Manoa. Her research is focused on the folding and function of proteins with complex topologies, utilizing both computational and experimental techniques to understand the molecular details of how proteins fold into biologically active molecules. She is inspired by how nature works and utilizes her multidisciplinary training to answer questions at the interface of chemistry, biology, and physics. Haglund received an M.S. in molecular biology and chemistry from Umeå University, Sweden and a Ph.D. in biochemistry and biophysics from Stockholm University, Sweden, and completed post doctoral training at Rice University and the at the University of California, San Diego.

Andrzej Kloczkowski

Member

Andrzej Kloczkowski is a Professor in the Department of Pediatrics at the Ohio State University, College of Medicine and Principal Investigator II at the Steve and Cindy Rasmussen Institute for Genomic Medicine at Nationwide Children's Hospital. Previously, he was Principal Investigator II at the Battelle Center for Mathematical Medicine at the Research Institute at Nationwide Children's Hospital. His research expertise is in computational biology and computational medicine. Kloczkowski received a Ph.D. in statistical thermodynamics from the Institute of Physical Chemistry of the Polish Academy of Sciences. He has served on the review panels for previous rounds of proposal evaluation for allocation of supercomputing time for the study of molecular dynamics.

Yun Lyna Luo

Member

Lyna Luo is an Associate Professor at Western University of Health Sciences and currently serves as an external editor of Nature - Communication Biology and as a co-chair of the Biophysical Society subgroup and ACS Molecular Mechanics session. Her research group focuses on developing and applying computational biophysics and chemistry methods to understand ion channel gating (e.g., PEIZO, Connexin, HCN channels), small molecular permeation, reversible-covalent binding, and protein allostery. She obtained her M.S. and Ph.D. from Zhejiang University in China and University of Paris VI in France, and subsequently received her postdoc training at the University of Chicago and at the Leadership Computing Facility at Argonne National Laboratory.

C. Denise Okafor

Member

Denise Okafor is an assistant professor in the Department of Biochemistry and Molecular Biology at Pennsylvania State University. Her lab uses molecular dynamics simulations and biochemical experiments to understand how structural properties of nuclear receptor ligands dictate transcriptional outcomes. She is a recipient of the Burroughs Wellcome Fund Career award at the scientific interface, an NSF CAREER award, NIH Director’s New Innovator Award, and the AAAS Marion Mason award. Okafor received a B.S. in biomedical chemistry from Oral Roberts University, and an M.S. in chemistry and a Ph.D. in biochemistry from the Georgia Institute of Technology. She performed postdoctoral research at Emory University working on nuclear receptors, a family of ligand-regulated transcription factors.

Steven W. Rick

Member

Steven Rick is a University Research Professor in the chemistry department at the University of New Orleans. Prior to his current position, he was a staff scientist at the National Cancer Institute. His research primarily focuses on using all-atom molecular dynamics simulations to study aqueous solutions, proteins, and polymers. He is also involved in the development of potential models, including those that treat many-body effects like polarization and charge transfer, and the development of sampling methods. Rick received a B.S. from the University of California, Los Angeles and Ph.D. from the University of California, Berkeley. He completed postdoctoral training at Brown University and Columbia University. He has served on the review panels for previous rounds of proposal evaluation for allocation of supercomputing time for the study of molecular dynamics.

Leonor Saiz

Member

Leonor Saiz is a Professor in the Biomedical Engineering Department at the University of California, Davis. Her research focuses on the dynamics of biological networks at the cellular and molecular level. Her lab combines computational and theoretical approaches with experimental data to understand how the observed behavior arises from the interactions and physical properties of the cellular components; and to infer detailed molecular properties, such as the in vivo DNA mechanics, from the cellular physiology. The ultimate goal of her work is to understand and follow the impact of molecular perturbations in the cellular components, such as a mutation in a protein or interventions with small molecules or drugs, through the different levels of biological organization up to the cellular and population behavior; one of the major challenges of modern biomedical sciences. Saiz received a Ph.D. in physics from the University of Barcelona, Spain.

Janani Sampath

Member

Janani Sampath is an Assistant Professor of Chemical Engineering at the University of Florida. Her expertise lies in using molecular dynamics simulations to understand the behavior of polymers, proteins, and their hybrids. Her group uses a combination of coarse grained and atomistic models to study systems ranging from synthetic polymer membranes, polymer-protein bioconjugate self-assembly, and polymers for therapeutic applications. Sampath received a Ph.D. in chemical engineering from the Ohio State University and completed postdoctoral training at the University of Washington and the Pacific Northwest National Laboratory.

David Sept

Member

David Sept is Professor of Biomedical Engineering and Associate Dean in the Rackham Graduate School at the University of Michigan. He was previously on the faculty at Washington University in St. Louis. Sept is an expert in biomolecular simulation and mathematical modeling. His work focuses on three primary areas: the dynamics and regulation of the cytoskeleton, the design and development of therapeutic agents that target the cytoskeleton, and multiscale modeling of biological polymers. He is a Fellow of the American Institute for Medical and Biological Engineering and an Associate Editor of Biophysical Journal. Sept received a Ph.D. in theoretical physics from the University of Alberta and completed postdoctoral training at the University of California, San Diego, and the Salk Institute for Biological Studies.

Arjun Sharma

Member

Arjun Sharma is an Assistant Professor of Biochemistry in the Department of Chemistry and Biochemistry at Purdue University Fort Wayne. His research focuses on molecular dynamics simulations of protein-protein and protein-ligand interactions, membrane channel protein gating mechanisms, de novo protein design, and multi-scale modeling of large protein complexes. He also studies amphiphilic polymer compounds and their applications in drug delivery, particularly in the formation and behavior of micelles. Sharma is a member of several professional societies, including the American Chemical Society, the Biochemical Society, the American Association of Pharmaceutical Sciences, and the Indiana Academy of Sciences. Sharma received an M.S. and Ph.D. in chemistry from the University of New Orleans and completed post-doctoral training at Lehigh University and the University of Vermont.

Lela Vukovic

Member

Lela Vukovic is an Associate Professor in the Department of Chemistry and Biochemistry at the University of Texas at El Paso. Her research interests involve developing and applying computational approaches with a focus on the design of molecules with high-affinity binding to biomolecules and synthetic materials, and the design and characterization of biomolecule-nanomaterial conjugates for biomedical applications. Vukovic received a B.Sc. and Ph.D. in chemistry from the University of Illinois at Chicago and was a visiting researcher at the Max Planck Institute for Biophysical Chemistry and a postdoctoral fellow at the NSF Center for the Physics of Living Cells at the University of Illinois Urbana-Champaign.

Feng Wang

Member

Feng Wang is a distinguished professor and Charles E. and Clydene Scharlau Endowed Professor in the department of Chemistry and Biochemistry at the University of Arkansas, Fayetteville. His research is related to the development of force fields to model intermolecular interactions based on accurate quantum mechanics equations. He is a recipient of an NSF CAREER Award. Wang received a B.S. in chemistry (honors) from Peking University, China, and a Ph. D. in theoretical chemistry from the University of Pittsburgh.