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Dilip N. Asthagiri

Current Position

Oak Ridge National Laboratory

2022–Present Senior Biomedical Staff Scientist, National Center for Computational Sciences

Rice University (courtesy appointment)

2022–Present Adjunct Associate Research Professor

Research Interests

Molecular Biophysics and Theoretical Chemistry. Molecular & Statistical Thermodynamics of Liquids and Bio-macromolecules, Hydration, Protein Stability and Conformation, NMR relaxation, (multiscale) Computer Simulations, Bayesian Statistical Analysis and Modeling.

Education

Indian Institute of Technology — Madras

1988–1992 B.Tech. Chemical Engineering

University of Michigan — Ann Arbor

1992–1994 M.S. Chemical Engineering

University of Delaware — Newark

1994–1999 Ph.D. Chemical Engineering (Mentor: Abraham M. Lenhoff)

Minor: Theoretical Chemistry

Thesis: *Modeling protein interactions in solution*

Previous Positions

Scripps Research Institute

1999–2002 Postdoc (Mentor: Donald Bashford), Department of Molecular Biology

Los Alamos National Laboratory

2002–2005 Postdoc (Mentor: Lawrence Pratt), Theoretical Chemistry and Molecular Physics

2005–2006 Technical Staff Member, Theoretical Chemistry and Molecular Physics

Johns Hopkins University

2006–2013 Assistant Professor, Chemical and Biomolecular Engineering

University of Texas Medical Branch

2013-2014 Visiting Scientist, Sealy Center for Structural Biology and Molecular Biophysics

Rice University

2014-2019 Director MChE Program & Senior Research Scientist, Chemical and Biomolecular Engineering

2019-2022 Associate Research Professor, Chemical and Biomolecular Engineering

Awards & Recognition

1989-1989	Merit Scholarship (for students with financial need)	*IIT-Madras*
1995	Garrett Reed Cantwell Scholarship (given to the top 1^{st} yr student)	*Chem. Eng. UD*
1999	University Competitive Fellowship (given to top students across disciplines)	*UD*
2011	Keenan Award (to support innovations in teaching)	*JHU*
2021	Best Fundamental Paper — South Texas Section of AIChE	*Rice*

Advising

Ph.D. Students Supervised	Safir S. Merchant (JHU, 2011; Facebook), Purushottam D. Dixit (JHU, 2011; faculty, Physics@UF Gainesville), Dheeraj S. Tomar (JHU, 2014; Xilio Therapeutics)
Ph.D. Students co-supervised	M. Hamsa Priya (Ohio State University, 2011; faculty, IIT-Madras), Arjun Valiya Parambathu (Rice, 2022; postdoc, U. Delaware), Yousef Alhashimi (Rice, expected 2023), Rohan Shridhar (Rice, expected 2023), Thiago Pinheiro (Rice, expected 2024)
Ph.D. Students closely worked with	Amit Paliwal (JHU, 2005; Intel), Artee Bansal (Rice, 2017; Aviva), Mohamed Al-Hosani (Rice, 2020; ADNOC)
Postdocs	Jindal Shah (JHU, 2006-2007, co-supervised; faculty, Oklahoma State)
UG research interns	Jeremy Harris (JHU, Summer/Fall 2007; BS 2008), Stephen Reilly (JHU, Fall 2008–Fall 2009; BS 2010), Jonathan White (JHU, Jan 2011–Dec 2011; BS 2012), Kelsey Dean (JHU, Fall 2010–Fall 2011; BS 2012), Niral Ramesh (Rice, Fall 2017–Fall 2018: BS 2019)
High school research interns	Parth Mathuria (August 2014–Jan 2016, Kempner High School), Prasanna Raparti (Summer 2017, Tompkins High School), Cristina Wyatt (Summer 2017, Episcopal High School), Kesavan Srivilliputhur (August 2018–March 2019, Denton High School), Samik Krishnan (Jan 2022-August 2022), Advika Sadasivan (May 2022-August 2022)

Courses Taught

Rice University

2021–Present	CHBE 302, Applied Mathematics and Numerical Methods for Chemical Engineers (UG)
2018–Present	CHBE 505, Advanced Numerical Methods (G)
2019	CHBE 470, Process Dynamics and Control (UG)
2014–2020	CHBE 303, Computer Programming in Chemical Engineering (UG)
2015	CHBE 305, Computational Methods in Chemical Engineering (UG)
2016	CHBE 412, Thermodynamics II (UG)
2017–2021	CHBE 611, Advanced Thermodynamics (G)

Johns Hopkins University

2006–2012	CHE 530, Thermodynamics and Statistical Mechanics (G)
2008–2012	CHE 305, Modeling and Statistical Analysis of Data (UG)

Research Highlights

Statistical mechanics of solvation

Contributed to developing the modern quasichemical theory of solutions. With my students, I showed that the quasichemical organization of the potential distribution theorem can be based on different order parameters, with each choice amounting to a different way of regularizing free energy calculations. Our work elucidated the relation between the solvation states of the solute, its interaction with the solvent, and the density fluctuations of the solvent at the scale of the solvation shell [34,35,45]. Our theory provides a rigorous framework to understand and interpret solvent effects in chemistry and biology [85].

Protein hydration

Our framework enabled the first all-atom calculation of the hydration thermodynamics of a realistic protein, cytochrome C [49]. Subsequent studies not only revealed the limitations of group additivity in interpreting protein hydration [51,54] but also highlighted the decisive role played by hydrophilic effects [56,66]. The culmination of this line of research led to the surprising discovery that for a protein temperature signatures of hydration that have been attributed to hydrophobic hydration instead arise from hydrophilic effects [83].

Classical & *Ab initio* simulations

The regularization approach enabled the direct calculation of hydration thermodynamics from *ab initio* simulations [38,47], avoiding unphysical solute states that can bedevil quantum chemical calculations. Our studies emphasize the need to understand the role of nuclear quantum motion in the physics of water and in the phenomena of solvation. Our work also reveals an unexpected connection between system size dependence of density fluctuations and its consequence for molecular simulations of hydration, especially of macromolecules [77].

Ions in biology

Our studies led to the discovery that only a small subset of water molecules in the first hydration shell sense the type of the ion [34,35]. Our work elucidated the importance of the bulk solvent in the hydration structure and thermodynamics of soft-ions or its lack of importance in the hydration of hard ions. These studies open an avenue to explore Hofmeister effects and ion-selectivity in (bio)molecular structures [33,40,44,46].

Protein-protein interactions

I developed a model to predict the osmotic second virial coefficient, B_{22}, of protein solutions with full account of the molecular structure [2,3]. Our work led to the discovery that a small number of high complementarity configurations determine the macroscopic B_{22}. Strongly bound water-of-hydration can either disrupt or facilitate the formation of high complementarity configurations and hence also affect the B_{22} [21,22].

Biological networks

The cellular expression of (bio)macromolecules provides insights into inter-relationships between the molecules. I contributed to developing an information entropy-based measure to characterize microarray expression data for microRNAs. This work led to the finding of "bio-markers" of potential importance in breast cancer [55].

NMR relaxation

Using atomistic simulation we calculated NMR T_1 and T_2 for bulk and confined fluids. Our work shows that the traditional models of inter- and intra-molecular relaxation are inadequate [63]. This line of research leads to the finding that nano-confinement and not paramagnetism is the basis of deviations from the traditional theories for alkanes in polymers [79]. Our work suggests the possibility of interpreting NMR relaxation in terms of relaxation of molecular modes [82], a step that can aid NMR studies in oil-and-gas exploration and in MRI. Recent work focuses on electron paramagnetic effects in the presence of Gd^{3+}(aq), a common contrast agent in MRI [86].

Publications

Metrics Google Scholar: 4200+ citations; $h = 36$

Book Chapter (Peer reviewed)

1. L. R. Pratt and D. Asthagiri, "Free energy calculations: theory and applications in chemistry and biology", in , Vol. 86 Springer Series in Chemical Physics, edited by Ch. Chipot and A. Pohorille (Springer, 2007) Chap. Potential distribution methods and free energy models of molecular solutions, pp. 323–351, DOI: 10.1007/978-3-540-38448-9_9.

Journal Articles

88. D. T. Gomez, L. R. Pratt, D. N. Asthagiri, and S. B. Rempe, "Hydrated anions: From clusters to bulk solution with quasi-chemical theory", Acc. Chem. Res. **55**, 2201–2212 (2022) DOI: 10.1021/acs.accounts.2c00078.

87. A. V. Parambathu, T. J. P. dos Santos, W. G. Chapman, and D. N. Asthagiri, "Comment on 'Calculation of solid–fluid interfacial free energy with consideration of solid deformation by molecular dynamics'", J. Phys. Chem. A **126**, 1782–1783 (2022) DOI: 10.1021/acs.jpca.1c07474.

86. P. M. Singer, A. V. Parambathu, T. P. dos Santos, Y. Liu, L. Alemany, G. H. Hirasaki, W. G. Chapman, and D. Asthagiri, "Predicting ^{1}H NMR relaxation in Gd^{3+}-aqua using molecular dynamics simulations", Phys. Chem. Chem. Phys. **23**, 20974–20984 (2021) DOI: 10.1039/D1CP03356E.

85. D. N. Asthagiri, M. E. Paulaitis, and L. R. Pratt, "Thermodynamics of hydration from the perspective of the molecular quasichemical theory of solutions (Invited Perspective)", JPCB **125**, 8294–8304 (2021) DOI: 10.1021/acs.jpcb.1c04182.

84. H. S. Ashbaugh, D. Asthagiri, T. L. Beck, and S. B. Rempe, "Tribute to Lawrence R. Pratt", JPCB **125**, 4925–4927 (2021) DOI: 10.1021/acs.jpcb.1c03298.

83. D. S. Tomar, M. E. Paulaitis, L. R. Pratt, and D. N. Asthagiri, "Hydrophilic interactions dominate the inverse temperature dependence of polypeptide hydration free energies attributed to hydrophobicity", J. Phys. Chem. Lett. **11**, 9965–9970 (2020) DOI: 10.1021/acs.jpclett.0c02972.

82. M. Alhosani, D. Asthagiri, M. Puerto, and W. G. Chapman, "Insights into the mechanisms affecting water/oil interfacial tension as a function of salt types and concentrations", Fluid Phase Eql. **522**, 112771 (2020) DOI: 10.1016/j.fluid.2020.112771.

81. D. Asthagiri, W. G. Chapman, G. J. Hirasaki, and P. M. Singer, "NMR ^{1}H-^{1}H dipole relaxation in fluids: Relaxation of individual ^{1}H-^{1}H pairs versus relaxation of molecular modes", J. Phys. Chem. B **124**, 10802–10810 (2020) DOI: 10.1021/acs.jpcb.0c08078.

80. D. Roush, D. Asthagiri, D. K. Babi, S. Benner, C. Bilodeau, G. Carta, P. Ernst, M. Fedesco, S. Fitzgibbon, M. Flamm, J. Griesbach, T. Grosskopf, E. B. Hansen, T. Hahn, S. Hunt, F. Insaidoo, A. M. Lenhoff, J. Lin, H. Marke, B. Marques, E. Papadakis, F. Schlegel, A. Staby, M. Stenvang, L. Sun, P. M. Tessier, R. Todd, E. von Lieres, J. Welsh, R. Willson, G. Wang, T. Wucherpfennig, and O. Zavalov, "Toward *in silico* CMC: An industrial collaborative approach to model-based process development", Biotech. Bioeng., 1000–1010 (2020) DOI: 10.1002/bit.27520.

79. P. M. Singer, A. V. Parambathu, X. Wang, D. Asthagiri, W. G. Chapman, G. J. Hirasaki, and M. Fleury, "Elucidating the ^{1}H NMR relaxation mechanism in polydisperse polymers and bitumen using measurements, MD simulations, and models", J. Phys. Chem. B **124**, 4222–4233 (2020) DOI: 10.1021/acs.jpcb.0c01941.

78. A. V. Parambathu, P. M. Singer, G. J. Hirasaki, W. G. Chapman, and D. Asthagiri, "Critical role of confinement in the NMR surface relaxation and diffusion of n-heptane in a polymer matrix revealed by MD simulations", J. Phys. Chem. B **124**, 3801–3810 (2020) DOI: 10.1021/acs.jpcb.0c00711.

77. D. Asthagiri and D. S. Tomar, "System size dependence of hydration-shell occupancy and its implications for assessing the hydrophobic and hydrophilic contributions to hydration", J. Phys. Chem. B **124**, 798–806 (2020) DOI: 10.1021/acs.jpcb.9b11200.

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75. D. S. Tomar, N. Ramesh, and D. Asthagiri, "Solvophobic and solvophilic contributions in the water-to-aqueous guanidinium chloride transfer free energy of model peptides", J. Chem. Phys. **148**, 222822 (2018) DOI: 10.1063/1.5022465, [• Invited article for special issue on "Ions in water"].

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68. A. Bansal, W. G. Chapman, and D. Asthagiri, "Quasichemical theory and the description of associating fluids relative to a reference: multiple bonding of a single site solute", J. Chem. Phys. **147**, 124505 (2017) DOI: 10.1063/1.4997663.

67. A. Bansal, W. G. Chapman, and D. Asthagiri, "Erratum: "Quasichemical theory and the description of associating fluids relative to a reference: multiple bonding of a single site solute" [J. Chem. Phys. 147, 124505 (2017)", J. Chem. Phys. **147**, 199901 (2017) DOI: 10.1063/1.5009414.

66. D. Asthagiri, D. Karandur, D. S. Tomar, and B. M. Pettitt, "Intramolecular interactions overcome hydration to drive the collapse transition of Gly_{15}", J. Phys. Chem. B **121**, 8078–8084 (2017) DOI: 10.1021/acs.jpcb.7b05469.

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64. A. Bansal, A. Valiya Parambathu, D. Asthagiri, K. R. Cox, and W. G. Chapman, "Thermodynamics of mixtures of patchy and spherical colloids of different sizes: A multi-body association theory with complete reference fluid information", J. Chem. Phys. **146**, 164904 (2017) DOI: 10.1063/1.4981913.

63. P. M. Singer, D. Asthagiri, W. G. Chapman, and G. J. Hirasaki, "Molecular dynamics simulations of NMR relaxation and diffusion of bulk hydrocarbons and water", J. Magn. Reson. **277**, 15–24 (2017) DOI: 10.1016/j.jmr.2017.02.001, [• Highlighted on Eureka Alert of the AAAS].

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61. A. Bansal, D. Asthagiri, K. R. Cox, and W. G. Chapman, "Structure and thermodynamics of a mixture of patchy and spherical colloids: A multi-body association theory with complete reference fluid information", J. Chem. Phys. **145**, 074904 (2016) DOI: 10.1063/1.4960985.

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58. D. Asthagiri, D. Ballal, P. Venkataraman, W. A. Fouad, K. R. Cox, and W. G. Chapman, "Response to "Comment on 'Isolating the non-polar contributions to the intermolecular potential for water-alkane interactions"' [J. Chem. Phys. 144, 137101 (2016)]", J. Chem. Phys. **144**, 137102 (2016) DOI: 10.1063/1.4944979.

57. M. I. Chaudhari, S. B. Rempe, D. Asthagiri, L. Tan, and L. R. Pratt, "Molecular theory and the effects of solute attractive forces on hydrophobic interactions", J. Phys. Chem. B **120**, 1864–1870 (2016) DOI: 10.1021/acs.jpcb.5b09552.

56. D. S. Tomar, V. Weber, B. M. Pettitt, and D. Asthagiri, "Importance of hydrophilic hydration and intramolecular interactions in the thermodynamics of Helix-Coil transition and Helix-Helix assembly in a deca-alanine peptide", J. Phys. Chem. B **120**, 69–76 (2016) DOI: 10.1021/acs.jpcb.5b09881, [• Highlighted in the special virtual issue of JPC-B (Biophysics), Feb. 2017].

55. N. Guzman, K. Agarwal, D. Asthagiri, L. Yu, M. Saji, M. D. Ringel, and M. E. Paulaitis, "Breast cancer-specific miR signature unique to extracellular vesicles includes "microRNA-like" tRNA fragments", Mol. Cancer Res. **13**, 891–901 (2015) DOI: 10.1158/1541-7786.MCR-14-0533, [• Featured on journal's research highlights page].

54. D. Tomar, V. Weber, B. M. Pettitt, and D. Asthagiri, "Conditional solvation thermodynamics of isoleucine in model peptides and the limitations of the group-transfer model", J. Phys. Chem. B **118**, 4080–4087 (2014) DOI: 10.1021/jp500727u.

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51. D. S. Tomar, D. Asthagiri, and V. Weber, "Solvation free energy of the peptide group: Its model dependence and implications for the additive-transfer free-energy model of protein stability", Biophys. J. **105**, 1482–1490 (2013) DOI: 10.1016/j.bpj.2013.08.011.

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8. D. Asthagiri and D. Bashford, "Continuum and atomistic modeling of ion partitioning into a peptide nanotube", Biophys. J. **82**, 1176–1189 (2002) DOI: 10.1016/S0006-3495(02)75475-1.

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1. D. Asthagiri and A. M. Lenhoff, "Influence of structural details in modeling electrostatically driven protein adsorption", Langmuir **13**, 6761–6768 (1997) DOI: 10.1021/la970608u.

Presentations

Invited

1. "Atomistic modeling of hydrophilic and hydrophobic contributions in protein solution thermodynamics", Advanced Computing for Life Sciences and Engineering Group, ORNL, (February, 2022).
2. "Thermodynamics of hydration from the perspective of the molecular quasichemical theory: From aqueous ions to hydrated proteins", ATOMS (Applied Thermodynamics and Molecular Simulation) Group, Federal University of Rio de Janeiro, Brazil, (September, 2021).
   URL: https://www.youtube.com/watch?v=dY92z_H7usA
3. "A reassessment of the thermodynamic forces that stabilize folded protein conformations in aqueous solutions", Multiscale Modeling of Biologics Drugs Symposium (Schrödinger / University of Delaware online seminar series), (February, 2021).
4. "Computer modeling of hydrophilic and hydrophobic contributions in protein solution thermodynamics — Prospects and Challenges", Symposium on Multiscale Modeling of Protein and Nucleic Acid Therapeutics, ACS National Meeting, San Francisco, CA (August 2020).
5. "Unraveling the molecular motions of viscous fluids and fluids under nano-confinement with NMR measurements and MD simulations" [co-presented with Dr. Philip Singer (Rice University)], Stelar/Eurelax webinar series on NMR Relaxometry Theory and Applications (July 2020)
6. "Molecular simulation of NMR relaxation behavior of fluids in polymer-alkane mixtures and model nano-porous systems: implications for understanding fluids in shale", NMR Today and Tomorrow: Downhole, at the Wellsite, and in the Lab, SPWLA NMR Special Interest Group Meeting, Spring, TX (June 2019).
7. "A quasichemical perspective of protein solution thermodynamics", 3$^{\mathrm{rd}}$ Modeling Workshop, Merck & Co., Inc. Kenilworth, NJ (May 2019).
8. "Molecular Dynamics Simulations of NMR Relaxation: Concepts and Applications to Hydrocarbons and Water in Confined Systems", Highlights from the 20$^{\mathrm{th}}$ Symposium on Thermophysical Properties, NIST; AIChE Annual Meeting (2018).
9. "Nano-pore confinement of hydrocarbons: a computational chemistry study integrated with NMR measurements", Schlumberger, Houston, TX (2017).
10. "Models of ion hydration: From molecular insights to an equation of state", Telluride Workshop on Ion hydration, Telluride, CO (2016).
11. "Hydrophobic and hydrophilic contributions in the folding of model polypeptides", Telluride Workshop on Ion hydration, Telluride, CO (2014).
12. "Protein solvation and the role of osmolytes — A quasichemical perspective", Indian Institute of Technology, Mumbai, India (2013).
13. "Protein solvation and the role of osmolytes — A quasichemical perspective", University of Texas Medical Branch, Galveston, TX (2013).
14. "Thermodynamics of protein folding and stability — A quasichemical perspective", University of Illinois-Chicago, IL (2013).
15. "Quasichemical consideration of the effect of osmolytes in protein solution thermodynamics", Bard College, NY (2013).
16. "Quasichemical consideration of the effects of osmolytes in protein solution thermodynamics", University of Tennessee, Knoxville, TN (2012).
17. "Quasichemical consideration of osmoylte-effects in protein solution thermodynamics", Telluride Workshop on Ion hydration, Telluride, CO (2012).
18. "Molecular foundations of ion selectivity in proteins", Department of Chemical and Biomolecular

Engineering, University of Houston, TX (2011).

19. "Statistical mechanics of ion selectivity in the KcsA potassium channel", Department of Chemical and Biomolecular Engineering, Tulane University, LA (2010).
20. "Building the solvent around the solute—A molecular *aufbau* approach to hydration", Telluride Workshop on Ion hydration, Telluride, CO (2010).
21. "Multi-state models of ion hydration and ion protein interactions", Department of Chemical and Biomolecular Engineering, Ohio State University, OH (2010).
22. "Potential distribution theorem and hydration thermodynamics", Michael Fisher Informal Statistical Physics Seminar Series, IPST, University of Maryland, MD (2008).
23. "Role of fluctuations in a snug-fit mechanism of KcsA channel selectivity", ACS Annual Meeting, Boston, MA (2007).
24. "Metals in biology: Tying chemistry to thermodynamics in bio-molecular systems", Department of Chemistry, Mt. Holyoke College, MA (2007).
25. "Metals in biology: Tying chemistry to thermodynamics in bio-molecular systems", Department of Chemical & Biomolecular Engineering, Johns Hopkins University, MD (2005).
26. "Continuum and atomistic modeling of ion partitioning into a peptide nanotube", Theoretical Chemistry & Molecular Physics Group, Los Alamos National Laboratory, Los Alamos, NM (Dec 2001).
27. "Molecular determinants of the osmotic second virial coefficient of protein solutions", NIDDK, National Institutes of Health, Bethesda, MD (Aug 2000).
28. "Modeling protein solution thermodynamics", Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA (Jan 1999).

Grantsmanship

Rice University

$25,731	Rice University Creative Ventures Fund (2022) Improving MRI contrast agents through molecular simulations and measurements (Role: PI)
$85,000	Chevron (2022) Effects of nano-confinement on the NMR response of fluids in organic shales using MD simulations (Role: coPI)
$2,136,180	National Science Foundation (2021-2027) Collaborative Research: Improving access to career and educational development (I-ACED). (Role: Senior Personnel. For this multi-PI, multi-institution effort, I lead the efforts to recruit, mentor, and train Master's students in Chemical Engineering)
$85,000	Chevron (2021) Effects of nano-pore confinement on the hydrocarbon storage and fracture properties of organic matter; a computational chemistry study integrated with NMR measurements (Role: coPI)
$231,000	Chevron (2017—2020) Effects of nano-pore confinement on the hydrocarbon storage and fracture properties of organic matter; a computational chemistry study integrated with NMR measurements (Role: Senior Scientist)
$110,000	ACS-PRF (2017—2019) Effects of nano-pore confinement on the hydrocarbon storage and fracture properties of organic matter; a computational chemistry study integrated with NMR measurements (Role: Senior Scientist)
$50,000	Rice Energy and Environment Initiative (2018–2019) Workflow to establish total gas in place in organic shale (Role: Senior Scientist)

Johns Hopkins University

$1,997,219	NSF-EFRI (2007—2011) An Integrated Computational and Experimental Model for Biochemical and Electrical Interactions in Ion Channels and the Impact of Sialic Acid on Neuronal Function (Role: coPI; As coPI received $250,000; funds helped to train 1.5 students on statistical mechanical theory, large scale simulations, and analysis of dynamics and thermodynamics of ion channels)
$50,000	ACS-PRF (2008—2011) Molecular basis of tetrahydrofuran-induced enclathration (Role: PI)

Computer time at NERSC and TACC (PI on all awards)

315,000 hrs	Studies on ion channel selectivity and voltage gating (2009—2011)
30,000 hrs	*Ab initio* studies of ion-hydration thermodynamics (2011)
200,000 hrs	Protein stability and protein-protein interactions in ionic liquids (2012)
192,000 hrs	Molecular scale studies on aqueous solutions, corrosion, and corrosion inhibitors (2012—2017)
150,000 hrs	TACC: Thermodynamics of protein folding (2013)

4200 node hrs	TACC: Effects of nano-pore confinement on the hydrocarbon storage and fracture properties of organic matter: a computational chemistry study integrated with NMR measurements (2018—2021)
350,000 hrs	Effects of nano-pore confinement on the hydrocarbon storage and fracture properties of organic matter: a computational chemistry study integrated with NMR measurements. Average award ≈116,000 hrs / yr (2017—2021)
1,810,000 hrs	Free energy calculations by regularizing binding energies. A framework for modeling ion- and osmolyte- specific effects in protein solution thermodynamics. Average award ≈260,000 hrs / yr (2012—2021)
6000 SUs	TACC: Free energies by regularizing binding energy distributions: Exploring the role of solvent on protein hydration (2022)
4000 SUs	TACC: Effects of nano-pore confinement on the hydrocarbon storage and fracture properties of organic matter: a computational chemistry study integrated with NMR measurements (2022)
100 GPU hrs; 150 CPU node hrs	Modeling solvent effects in biomolecular structure and phase behavior (2022)

Service

Departmental Service (Rice University)

2016–Present	Graduate Studies Committee
2016–Present	Graduate Admissions Committee

Departmental Service (Johns Hopkins University)

2007–2011	Graduate Admissions Committee
2008–2011	Departmental Seminar Committee

Organizing

2008–2012	Session chair/co-chair, Thermodynamics at the Nanoscale, AIChE Annual Meeting
2015	Organizing committee, Conference on 25 years of the Statistical Associating Fluid Theory
2015	Organizing committee, Gulf Coast Undergraduate Research Symposium

Professional Associations

Member, American Chemical Society (since 1994)

Member, Biophysical Society (since 2006)

Member, American Physical Society (since 2017)