

CURRICULUM VITAE

Ivaylo Ivanov, Ph.D.

Professor of Chemistry, Department of Chemistry, Georgia State University

P.O. Box 3965, Atlanta, GA 30302-3965

Email: iivanov@gsu.edu · Web: <https://ivanov-group.org> · ORCID: 0000-0002-5306-1005

EDUCATION

Ph.D. in Chemistry, 2004 – University of Pennsylvania, Philadelphia, PA

Dissertation: "Terascale Ab Initio Molecular Dynamics Simulations of Proton Transfer and Dissociation Processes in Chemical and Biological Systems"

M.S. in Chemistry, 1999 – Carnegie Mellon University, Pittsburgh, PA

B.S. in Chemistry, 1996 – Sofia University, Sofia, Bulgaria

PROFESSIONAL APPOINTMENTS

2020 – Present Professor, Georgia State University, Atlanta, GA
2015 – 2020 Associate Professor, Georgia State University, Atlanta, GA
2009 – 2015 Assistant Professor, Georgia State University, Atlanta, GA
2012 – Present Faculty, Center for Diagnostics & Therapeutics, Georgia State University
2009 – Present Faculty, Molecular Basis of Disease Program, Georgia State University
2005 – 2009 Postdoctoral Research Associate, University of California-San Diego, La Jolla, CA

PEER-REVIEWED PUBLICATIONS

Submitted and In Press

1. Serafim, L. F., Tsutakawa, S. E., Arvai, S. A., Kossmann, B. R., Mantha, A. K., Abbotts, R., Wilson III, D. M., Mitra, S., Tainer, J. A., & Ivanov, I.* Orchestrated metal ion repositioning defines the dynamic catalytic strategy of the essential DNA repair nuclease APE1. *bioRxiv* 724140 [Preprint]. May 14, 2026. doi:10.64898/2026.05.11.724140 (under review in *Nucleic Acids Research*).
2. Fasken, M. B., Leung, S. W., Serafim, L. F., Yan, C., Intemann, M. L., Gable, D. L., Barañano, K. W., Ivanov, I., Ghalei, H., & Corbett, A. H. Systematic comparison of pathogenic variants of the RNA exosome gene EXOSC3/RRP40 in *Saccharomyces cerevisiae* reveals variant-specific functional consequences. *bioRxiv* 741578 [Preprint]. August 2, 2026. doi:10.64898/2026.07.29.741578, PMID: PMC13484212. (under review in *Journal of Biological Chemistry*).

Published (72 publications, cited >4600 times in Google Scholar, h-index 40)

1. Syed, A., Serafim, L. F., Arvai, A. S., Minko, I. G., Tang, H. Y. H., Huffman, J. L., Mol, C. D., Hitomi, K., Sarker, A. H., Parikh, S., Tsai, S. L., Bacolla, A., Shin, D. S., Cunningham, R. P., Iwai, S., Chowdhury, D., Lloyd, R. S., Ivanov, I.* & Tainer, J. A.* A unified catalytic mechanism in bifunctional DNA glycosylases with an evolutionarily conserved aspartate-lysine dyad. *Nature Communications* 17, 8681 (2026). doi:10.1038/s41467-026-75471-1.
2. Kim, M., Jeong, E., Park, J., D'Souza, A., Tsai, M-S., Yan, C., Ivanov, I., Chazin, W. J., Kim, H. S., Schärer, O. D. The interaction of XPG with TFIIH through p62 and XPD is required for the completion of nucleotide excision repair. *Nucleic Acids Research* (2026) 54, gkag078, doi:10.1093/nar/gkag078.
3. Paul, T., Yan, C., Derdeyn-Blackwell, G. & Ivanov, I.* Translocation mechanism of xeroderma pigmentosum group D protein on single-stranded DNA and genetic disease etiology. *Nature Communications* (2025), 16, 11703, doi:10.1038/s41467-025-66834-1, PMID: 41315283, PMID: PMC12753804.

4. Fang, S., Zhou, L., Chen, G., Zhang, J., Wang, X., Jeong, I. H., Jacobs, S. E., Kossmann, B. R., Wei, W., Liu, S., Jeong, G. H., Xie, Y., Duong, D., Seyfried, N. T., Ivanov, I., Mabb, A. M., Kiyokawa, H., Zhao, B. & Yin, J. Engineering a cell-based orthogonal ubiquitin transfer cascade for profiling the substrates of RBR E3 Parkin. *iScience* (2025) 28, 112913, doi:10.1016/j.isci.2025.112913, PMID: PMC12271601.
5. Paul, T., Yan, C., Yu, J., Tsutakawa, S. E., Tainer, J. A., Wang, D. & Ivanov, I.* Molecular model of TFIIH recruitment to the transcription-coupled repair machinery. *Nature Communications* (2025) 16, 2341, doi:10.1038/s41467-025-57593-0, PMID: PMC11890784. (highlighted by the Oak Ridge Leadership Computing Facility)
6. Dang, T., EswarKumar, N., Tripathi, S. K., Yan, C., Wang, C. H., Cao, M., Paul, T. K., Agboluaje, E. O., Xiong, M. P., Ivanov, I., Ho, M. C. & Zheng, Y. G. Oligomerization of protein arginine methyltransferase 1 and its functional impact on substrate arginine methylation. *Journal of Biological Chemistry* (2024) 300, 107947, doi:10.1016/j.jbc.2024.107947, PMID: PMC11681865.
7. Yu, J., Yan, C., Paul, T., Brewer, L., Tsutakawa, S. E., Tsai, C. L., Hamdan, S. M., Tainer, J. A. & Ivanov, I.* Molecular architecture and functional dynamics of the pre-incision complex in nucleotide excision repair. *Nature Communications* (2024) 15, 8511, doi:10.1038/s41467-024-52860-y, PMID: PMC11445577. (highlighted by the Oak Ridge Leadership Computing Facility)
8. Chinnam, N. B., Thapar, R., Arvai, A. S., Sarker, A. H., Soll, J. M., Paul, T., Syed, A., Rosenberg, D. J., Hammel, M., Bacolla, A., Katsonis, P., Asthana, A., Tsai, M. S., Ivanov, I., Lichtarge, O., Silverman, R. H., Mosammamarast, N., Tsutakawa, S. E. & Tainer, J. A. ASCC1 structures and bioinformatics reveal a novel Helix-Clasp-Helix RNA-binding motif linked to a two-histidine phosphodiesterase. *Journal of Biological Chemistry* (2024) 300, 107368, doi:10.1016/j.jbc.2024.107368, PMID: PMC11214414.
9. Yu, J., Yan, C., Dodd, T., Tsai, C. L., Tainer, J. A., Tsutakawa, S. E. & Ivanov, I.* Dynamic conformational switching underlies TFIIH function in transcription and DNA repair and impacts genetic diseases. *Nature Communications* (2023) 14, 2758, doi:10.1038/s41467-023-38416-6, PMID: PMC10183003. (highlighted by the Oak Ridge Leadership Computing Facility)
10. Bralic, A., Tehseen, M., Sobhy, M. A., Tsai, C. L., Alhudhali, L., Yi, G., Yu, J., Yan, C., Ivanov, I., Tsutakawa, S. E., Tainer, J. A. & Hamdan, S. M. A scanning-to-incision switch in TFIIH-XPG induced by DNA damage licenses nucleotide excision repair. *Nucleic Acids Research* (2023) 51, 1019, doi:10.1093/nar/gkac1095, PMID: PMC9943652. (chosen as a breakthrough article by the NAR editors)
11. Yan, C., Dodd, T., Yu, J., Leung, B., Xu, J., Oh, J., Wang, D. & Ivanov, I.* Mechanism of Rad26-assisted rescue of stalled RNA polymerase II in transcription-coupled repair. *Nature Communications* (2021) 12, 7001, doi:10.1038/s41467-021-27295-4, PMID: PMC8636621. (highlighted by the Oak Ridge Leadership Computing Facility)
12. Dodd, T., Yao, X.-Q., Hamelberg, D., Ivanov, I.* Subsets of adjacent nodes (SOAN): A fast method for computing suboptimal paths in protein dynamic networks. *Molecular Physics* (2021) 119, e1893847, doi:10.1080/00268976.2021.1893847. (invited article for the Michael L. Klein special issue)
13. Dodd, T., Botto, M., Paul, F., Fernandez-Leiro, R., Lamers, M. H. & Ivanov, I.* Polymerization and editing modes of a high-fidelity DNA polymerase are linked by a well-defined path. *Nature Communications* (2020) 11, 5379, doi:10.1038/s41467-020-19165-2, PMID: PMC7584608. (highlighted by the Oak Ridge Leadership Computing Facility)
14. Qian, K., Yan, C., Su, H., Dang, T., Zhou, B., Wang, Z., Zhao, X., Ivanov, I., Ho, M. C. & Zheng, Y. G. Pharmacophore-based screening of diamidine small molecule inhibitors for protein arginine methyltransferases. *RSC Medicinal Chemistry* (2021) 12, 95, doi:10.1039/d0md00259c, PMID: PMC8130551.
15. Tsutakawa, S. E., Tsai, C. L., Yan, C., Bralic, A., Chazin, W. J., Hamdan, S. M., Schärer, O. D., Ivanov, I. & Tainer, J. A. Envisioning how the prototypic molecular machine TFIIH functions in transcription initiation and DNA repair. *DNA Repair (Amst)* (2020) 96, 102972, doi:10.1016/j.dnarep.2020.102972, PMID: PMC7669588.
16. Yuan, Z., Schneider, S., Dodd, T., Riera, A., Bai, L., Yan, C., Magdalou, I., Ivanov, I.*, Stillman, B., Li, H. & Speck, C. Structural mechanism of helicase loading onto replication origin DNA by ORC-CDC6.

- Proceedings of the National Academy of Sciences USA* (2020) 117, 17747, doi:10.1073/pnas.2006231117, PMCID: PMC7395460.
17. Dodd, T., Yan, C. & Ivanov, I.* Simulation-based methods for model building and refinement in cryoelectron microscopy. *Journal of Chemical Information and Modeling* (2020) 60, 2470, doi:10.1021/acs.jcim.0c00087, PMCID: PMC7284120.
 18. Yan, C., Dodd, T., He, Y., Tainer, J. A., Tsutakawa, S. E. & Ivanov, I.* Transcription preinitiation complex structure and dynamics provide insight into genetic diseases. *Nature Structural & Molecular Biology* (2019) 26, 397, doi:10.1038/s41594-019-0220-3, PMCID: PMC6642811. (recommended by Faculty of 1000 Prime; highlighted by the Oak Ridge Leadership Computing Facility; cited >100 times)
 19. Perumal, S. K., Xu, X., Yan, C., Ivanov, I.* & Benkovic, S. J. Recognition of a key anchor residue by a conserved hydrophobic pocket ensures subunit interface integrity in DNA clamps. *Journal of Molecular Biology* (2019) 431, 2493, doi:10.1016/j.jmb.2019.04.035, PMCID: PMC6527350.
 20. Carter, E. K., Laughlin-Toth, S., Dodd, T., Wilson, W. D. & Ivanov, I.* Small molecule binders recognize DNA microstructural variations via an induced fit mechanism. *Physical Chemistry Chemical Physics* (2019) 21, 1841, doi:10.1039/c8cp05537h, PMCID: PMC6497476.
 21. Han, Y., Yan, C., Fishbain, S., Ivanov, I. & He, Y. Structural visualization of RNA polymerase III transcription machineries. *Cell Discovery* (2018) 4, 40, doi:10.1038/s41421-018-0044-z, PMCID: PMC6066478.
 22. Dodd, T., Yan, C., Kossmann, B. R., Martin, K. & Ivanov, I.* Uncovering universal rules governing the selectivity of the archetypal DNA glycosylase TDG. *Proceedings of the National Academy of Sciences USA* (2018) 115, 5974, doi:10.1073/pnas.1803323115, PMCID: PMC6003370. (highlighted by the San Diego Supercomputer Center)
 23. Li, J., Li, S., Guo, J., Li, Q., Long, J., Ma, C., Ding, Y., Yan, C., Li, L., Wu, Z., Zhu, H., Li, K. K., Wen, L., Zhang, Q., Xue, Q., Zhao, C., Liu, N., Ivanov, I., Luo, M., Xi, R., Long, H., Wang, P. G. & Chen, Y. Natural product Micheliolide (MCL) irreversibly activates pyruvate kinase M2 and suppresses leukemia. *Journal of Medicinal Chemistry* (2018) 61, 4155, doi:10.1021/acs.jmedchem.8b00241, PMCID: PMC5949721. (cited >150 times)
 24. Han, Y., Yan, C., Nguyen, T. H. D., Jackobel, A. J., Ivanov, I., Knutson, B. A. & He, Y. Structural mechanism of ATP-independent transcription initiation by RNA polymerase I. *eLife* (2017) 6, e27414, doi:10.7554/eLife.27414, PMCID: PMC5489313.
 25. Rashid, F., Harris, P. D., Zaher, M. S., Sobhy, M. A., Joudeh, L. I., Yan, C., Piwonski, H., Tsutakawa, S. E., Ivanov, I., Tainer, J. A., Habuchi, S. & Hamdan, S. M. Single-molecule FRET unveils induced-fit mechanism for substrate selectivity in flap endonuclease 1. *eLife* (2017) 6, e21884, doi:10.7554/eLife.21884, PMCID: PMC5358979. (recommended by Faculty of 1000 Prime)
 26. Laughlin-Toth, S., Carter, E. K., Ivanov, I.* & Wilson, W. D. DNA microstructure influences selective binding of small molecules designed to target mixed-site DNA sequences. *Nucleic Acids Research* (2017) 45, 1297, doi:10.1093/nar/gkw1232, PMCID: PMC5388402.
 27. Zhang, J., Qian, K., Yan, C., He, M., Jassim, B. A., Ivanov, I. & Zheng, Y. G. Discovery of decamidine as a new and potent PRMT1 inhibitor. *Medicinal Chemistry Communications* (2017) 8, 440, doi:10.1039/c6md00573j, PMCID: PMC5477784.
 28. Turaga, R. C., Yin, L., Yang, J. J., Lee, H., Ivanov, I., Yan, C., Yang, H., Grossniklaus, H. E., Wang, S., Ma, C., Sun, L. & Liu, Z. R. Rational design of a protein that binds integrin α v β 3 outside the ligand binding site. *Nature Communications* (2016) 7, 11675, doi:10.1038/ncomms11675, PMCID: PMC4895024.
 29. Kossmann, B. R., Abdelmalak, M., Lopez, S., Tender, G., Yan, C., Pommier, Y., Marchand, C. & Ivanov, I.* Discovery of selective inhibitors of tyrosyl-DNA phosphodiesterase 2 by targeting the enzyme DNA-binding cleft. *Bioorganic and Medicinal Chemistry Letters* (2016) 26, 3232, doi:10.1016/j.bmcl.2016.05.065, PMCID: PMC4939481.

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31. Xu, X., Yan, C., Kossmann, B. R. & Ivanov, I.* Secondary interaction interfaces with PCNA control conformational switching of DNA polymerase PolB from polymerization to editing. *Journal of Physical Chemistry B* (2016) 120, 8379, doi:10.1021/acs.jpcc.6b02082, PMCID: PMC5001886. (Invited article for the J. Andrew McCammon Festschrift special issue)
32. Hudson, W. H., Kossmann, B. R., de Vera, I. M., Chuo, S. W., Weikum, E. R., Eick, G. N., Thornton, J. W., Ivanov, I., Kojetin, D. J. & Ortlund, E. A. Distal substitutions drive divergent DNA specificity among paralogous transcription factors through subdivision of conformational space. *Proceedings of the National Academy of Sciences USA* (2016) 113, 326, doi:10.1073/pnas.1518960113, PMCID: PMC4720311.
33. Musille, P. M., Kossmann, B. R., Kohn, J. A., Ivanov, I. & Ortlund, E. A. Unexpected allosteric network contributes to LRH-1 co-regulator selectivity. *Journal of Biological Chemistry* (2016) 291, 1411, doi:10.1074/jbc.M115.662874, PMCID: PMC4714224.
34. Xu, X., Yan, C., Wohlhueter, R. & Ivanov, I.* Integrative modeling of macromolecular assemblies from low to near-atomic resolution. *Computational and Structural Biotechnology Journal* (2015) 13, 492, doi:10.1016/j.csbj.2015.08.005, PMCID: PMC4588362.
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36. Tsutakawa, S. E., Yan, C., Xu, X., Weinacht, C. P., Freudenthal, B. D., Yang, K., Zhuang, Z., Washington, M. T., Tainer, J. A. & Ivanov, I.* Structurally distinct ubiquitin- and SUMO-modified PCNA: Implications for their distinct roles in the DNA damage response. *Structure* (2015) 23, 724, doi:10.1016/j.str.2015.02.008, PMCID: PMC4394044.
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38. Yan, L., Yan, C., Qian, K., Su, H., Kofsky-Wofford, S. A., Lee, W. C., Zhao, X., Ho, M. C., Ivanov, I.* & Zheng, Y. G. Diamidine compounds for selective inhibition of protein arginine methyltransferase 1. *Journal of Medicinal Chemistry* (2014) 57, 2611, doi:10.1021/jm401884z, PMCID: PMC3983339. (cited >100 times)
39. Xu, X., Guardiani, C., Yan, C. & Ivanov, I.* Opening pathways of the DNA clamps proliferating cell nuclear antigen and Rad9-Rad1-Hus1. *Nucleic Acids Research* (2013) 41, 10020, doi:10.1093/nar/gkt810, PMCID: PMC3905852.
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41. Tsutakawa, S. E., Shin, D. S., Mol, C. D., Izumi, T., Arvai, A. S., Mantha, A. K., Szczesny, B., Ivanov, I., Hosfield, D. J., Maiti, B., Pique, M. E., Frankel, K. A., Hitomi, K., Cunningham, R. P., Mitra, S. & Tainer, J. A. Conserved structural chemistry for incision activity in structurally non-homologous apurinic/apyrimidinic endonuclease APE1 and endonuclease IV DNA repair enzymes. *Journal of Biological Chemistry* (2013) 288, 8445, doi:10.1074/jbc.M112.422774, PMCID: PMC3605660. (cited >100 times)
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43. Ivanov, I.* Enzyme cofactors: Double-edged sword for catalysis. *Nature Chemistry* (2013) 5, 6, doi:10.1038/nchem.1529, PMID: 23247167.

44. Cheng, X. & Ivanov, I. Molecular dynamics. *Methods in Molecular Biology* (2012) 929, 243, doi:10.1007/978-1-62703-050-2_11, PMID: 23007433.
45. Querol-Audi, J., Yan, C., Xu, X., Tsutakawa, S. E., Tsai, M. S., Tainer, J. A., Cooper, P. K., Nogales, E. & Ivanov, I.* Repair complexes of FEN1 endonuclease, DNA, and Rad9-Hus1-Rad1 are distinguished from their PCNA counterparts by functionally important stability. *Proceedings of the National Academy of Sciences USA* (2012) 109, 8528, doi:10.1073/pnas.1121116109, PMCID: PMC3365210.
46. Tsutakawa, S. E., Van Wynsberghe, A. W., Freudenthal, B. D., Weinacht, C. P., Gakhar, L., Washington, M. T., Zhuang, Z., Tainer, J. A. & Ivanov, I.* Solution X-ray scattering combined with computational modeling reveals multiple conformations of covalently bound ubiquitin on PCNA. *Proceedings of the National Academy of Sciences USA* (2011) 108, 17672, doi:10.1073/pnas.1110480108, PMCID: PMC3203759. (recommended by Faculty of 1000 Prime; highlighted by the Oak Ridge Leadership Computing Facility)
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72. Ivanov, I., Gherman, B. F. & Yaron, D. Comparison of the INDO band structures of polyacetylene, polythiophene, polyfuran, and polypyrrole. *Synthetic Metals* (2001) 116, 111, doi:10.1016/s0379-6779(00)00526-9.

* denotes corresponding author.

RESEARCH FUNDING

Active

National Institute of Environmental Health Sciences R01 ES032786 (4/1/22 – 3/31/28); Title: “Integrative Modeling of Biomolecular Machinery in Nucleotide Excision Repair”; Role: Principal Investigator; Total cost: \$2,082,459

National Institute of General Medical Sciences R35 GM139382 (3/1/21 – 2/28/27); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation and DNA Repair”; Role: Principal Investigator; Total cost: \$2,261,126

National Cancer Institute P01 CA092584 (9/30/26 – 8/31/31); Title: “Structural Cell Biology of DNA Repair Machines”; Role: Senior Investigator; Total cost: \$395,749

Completed

National Cancer Institute P01 CA092584 (9/27/21 – 8/31/26); Title: “Structural Cell Biology of DNA Repair Machines”; Role: Senior Investigator; Total cost: \$275,000

National Science Foundation MCB-2027902 (8/1/20 – 7/31/25); Title: “Advanced Computational Modeling of Pathways for Epigenetic Regulation and Genome Maintenance”; Role: Principal Investigator; Total cost: \$765,882

National Cancer Institute P01 CA092584 (4/30/20 – 8/31/21); Title: “Structural Cell Biology of DNA Repair Machines”; Role: Subcontract PI; Total cost: \$85,000

National Institute of General Medical Sciences R01 GM110387 (9/1/15 – 8/31/21); Title: “Integrative Modeling of PCNA Assemblies Engaged in Genome Duplication and Repair”; Role: Principal Investigator; Total cost: \$1,675,000

Cleon C. Arrington Research Initiation Grant (7/1/18 – 6/30/19); Title: “Uncovering the Complex Interplay of DNA Repair and Epigenetic Regulation in Genome Maintenance”; Role: Principal Investigator; Total cost: \$20,000

National Institute of General Medical Sciences R01 GM126154 (4/1/18 – 12/31/21); Title: “Mechanism and Inhibition of Protein Arginine Methylation”; Role: Co-Investigator; Total cost: \$160,000 (to I.I.)

National Science Foundation CAREER Award MCB-1149521 (5/1/12 – 4/30/18); Title: “Modeling Assemblies and Interactions at the Replication Fork: Sliding Clamps and Clamp Loaders”; Role: Principal Investigator; Total cost: \$824,000

National Cancer Institute R01 CA118113 (6/1/14 – 5/31/19); Title: “p68 and Ca-Calmodulin Interaction in Cell Migration”; Role: Co-Investigator; Direct cost: \$40,000 (to I.I.)

Cleon C. Arrington Research Initiation Grant (2/1/11 – 6/30/12); Title: “Modeling Assemblies and Interactions in Eukaryotic Clamp Loading”; Role: Principal Investigator; Total cost: \$10,000

COMPUTATIONAL ALLOCATIONS AT NATIONAL SUPERCOMPUTING FACILITIES

1. Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award (1/1/26 – 12/31/26); Title: “Advanced Computational Modeling of Molecular Machines in Nucleotide Excision Repair”; Role: Principal Investigator; Awarded 400,000 service units at the Oak Ridge Leadership Computing Facility. The value of an INCITE award for a single project typically exceeds a million dollars.
2. INCITE Award (1/1/25 – 12/31/25); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation and DNA Repair”; Role: Principal Investigator; Awarded 400,000 service units at the Oak Ridge Leadership Computing Facility.
3. INCITE Award (1/1/24 – 12/31/24); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation and DNA Repair”; Role: Principal Investigator; Awarded 450,000 service units at the Oak Ridge Leadership Computing Facility.

4. INCITE Award (1/1/23 – 12/31/23); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation”; Role: Principal Investigator; Awarded 290,000 service units at the Oak Ridge Leadership Computing Facility. The INCITE Award provided access to Frontier, rated at the time the most powerful supercomputer in the world.
5. INCITE Award (1/1/22 – 12/31/22); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation”; Role: Principal Investigator; Awarded 190,000 service units at the Oak Ridge Leadership Computing Facility.
6. INCITE Award (1/1/21 – 12/31/21); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation”; Role: Principal Investigator; Awarded 260,000 service units at the Oak Ridge Leadership Computing Facility.
7. INCITE Award (1/1/20 – 12/31/20); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation and DNA Repair”; Role: Principal Investigator; Awarded 260,000 service units at the Oak Ridge Leadership Computing Facility.
8. INCITE Award (1/1/19 – 12/31/19); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation”; Role: Principal Investigator; Awarded 220,000 service units (>25 million CPU hours) at the Oak Ridge Leadership Computing Facility. The INCITE Award provided access to Summit, rated at the time the most powerful supercomputer in the world.
9. NSF/XSEDE program CHE110042 (10/1/14 – 3/31/20); Title: “Integrative Modeling of Complex Biological Assemblies”; Role: Principal Investigator; Awarded 17,372,000 CPU hours and >200,000 GPU node hours. The value of the awarded resources is \$560,604.
10. ERCAP DOE Award (1/7/16 – 1/5/19); Title: “Integrative Modeling of Protein/DNA Complexes at the Replication Fork”; Role: Principal Investigator; Awarded >10,000,000 CPU hours at the National Energy Research Scientific Computing Center.
11. ERCAP DOE Award (1/7/15 – 12/31/15); Title: “Integrative Modeling of Protein/DNA Complexes at the Replication Fork”; Role: Principal Investigator; Awarded 2,200,000 CPU hours at the National Energy Research Scientific Computing Center.
12. 2013 ASCR Leadership Computing Challenge Award (7/1/2013 – 12/31/2014); Title: “Exploring the Chemical Landscape for Base Excision DNA Repair”; Role: Principal Investigator; Awarded 3,000,000 CPU hours at the National Energy Research Scientific Computing Center.
13. NERSC Initiative for Scientific Exploration (NISE) Award (5/1/11 – 4/30/12); Title: “An Integrative Strategy to Model Complex Biological Assemblies”; Role: Principal Investigator; Awarded 960,000 CPU hours at the National Energy Research Scientific Computing Center.
14. INCITE Award BIP007 (1/1/09 – 12/31/10); Title: “Interplay of AAA+ Molecular Machines, DNA Repair Enzymes and Sliding Clamps at the Replication Fork: A Multiscale Approach to Modeling Replisome Assembly and Function”; Role: Principal Investigator; Awarded 6,500,000 CPU hours at the Oak Ridge Leadership Computing Facility.

HONORS AND AWARDS (SELECTED)

1. Innovative and Novel Computational Impact on Theory and Experiment (INCITE) award from the Department of Energy Office of Science (2010 and 2019–2026)
2. Cleon C. Arrington Research Initiation Grant from Georgia State University (2018)
3. ASCR Leadership Computing Challenge Award from the Department of Energy Office of Science (2013)
4. Dean’s Early Career Award from Georgia State University (2013)
5. CAREER Award from the National Science Foundation (2012)
6. NERSC Initiative for Scientific Exploration (NISE) Award from the Department of Energy Office of Science (2011)
7. Cleon C. Arrington Research Initiation Grant from Georgia State University (2011)
8. La Jolla Interfaces in Science Postdoctoral Fellowship, Burroughs Wellcome Fund (2005–2007)

9. Chemical Computing Group Excellence Award from the American Chemical Society (2003)
10. Chemistry Department Chairman's Award from the University of Pennsylvania (2000)
11. Chemistry Department Teaching Award from Carnegie Mellon University (1999)

RECOGNITION AND MEDIA COVERAGE

1. Coverage of a publication in Nature Communications (2025), doi:10.1038/s41467-025-57593-0. Altmetric score 36; 95th percentile (ranked 7,543rd) of 170,252 tracked articles of similar age in all journals and 85th percentile (ranked 205th) of 1,427 in Nature Communications. Featured by the Oak Ridge Leadership Computing Facility: "Summit supercomputer draws molecular blueprint for repairing damaged DNA."
2. Coverage of a publication in Nature Communications (2025), doi:10.1038/s41467-024-52860-y. Altmetric score 62; 97th percentile (ranked 9,419th) of 316,219 tracked articles of similar age in all journals and 85th percentile (ranked 340th) of 2,424 in Nature Communications. Featured by the Oak Ridge Leadership Computing Facility: "Summit supercomputer draws molecular blueprint for repairing damaged DNA."
3. Coverage of a publication in Nature Communications (2023), doi:10.1038/s41467-023-38416-6. Altmetric score 26; 92nd percentile (ranked 27,860) of 375,925 tracked articles of similar age in all journals and 68th percentile (ranked 631) of 2,034 in Nature Communications. Featured by the Oak Ridge Leadership Computing Facility: "New Insights into a Shapeshifting Protein Complex."
4. Coverage of a publication in Nature Communications (2021), doi:10.1038/s41467-021-27295-4. Featured by the Oak Ridge Leadership Computing Facility: "Decoding the Role of CSB Protein in DNA Repair."
5. Coverage of a publication in Nature Communications (2020), doi:10.1038/s41467-020-19165-2. Altmetric score 17; 87th percentile (ranked 53,523) of 419,570 tracked articles of similar age in all journals and 46th percentile (ranked 918) of 1,710 in Nature Communications. Featured by the Oak Ridge Leadership Computing Facility: "Simulations Reveal Nature's Design for Error Correction During DNA Replication."
6. Coverage of a publication in Nature Structural & Molecular Biology (2019), doi:10.1038/s41594-019-0220-3. Altmetric score 63; 96th percentile (ranked 4,371) of 118,590 tracked articles of similar age in all journals and 85th percentile (ranked 2) of 14 in Nature Structural & Molecular Biology. Featured by the Oak Ridge Leadership Computing Facility: "Summit Charts a Course to Uncover the Origins of Genetic Diseases."
7. Coverage of a publication in Proceedings of the National Academy of Sciences (2018), doi:10.1073/pnas.1803323115. Featured by the San Diego Supercomputer Center: "How an Enzyme Repairs DNA via a Pinch-Push-Pull Mechanism." Highlighted by Scientific Computing Online, Primeur Magazine, HealthNewsDigest.com, Newswise and Publicnow.
8. Coverage of a publication in Nature (2016), doi:10.1038/nature17970. Altmetric score 135; 98th percentile (ranked 3,654) of 227,366 tracked articles of similar age in all journals and 60th percentile (ranked 388) of 975 in Nature. Highlighted by Science360, the MCB Division of the NSF, Phys.org, Technology.org, e!Science News, Nanowerk, Bioportfolio, EurekAlert!, Newswise and Science Daily; featured by the Texas Advanced Computing Center: "How to See Living Machines."
9. Coverage of a publication in Nature Communications (2016), doi:10.1038/ncomms11675. Altmetric score 201; 99th percentile (ranked 1,781) of 190,421 tracked articles of similar age in all journals and 94th percentile (ranked 37) of 713 in Nature Communications.
10. Coverage of a publication in Proceedings of the National Academy of Sciences (2016), doi:10.1073/pnas.1518960113. Altmetric score 51; 96th percentile of 252,241 tracked articles of similar age in all journals and 76th percentile (ranked 238) of 1,024 in PNAS. Highlighted by ScienceDaily, Health Medicine Network, PhysOrg.com and EurekAlert!

11. Coverage of a publication in Proceedings of the National Academy of Sciences (2011), doi:10.1073/pnas.1110480108. Featured science highlight “Researchers Show How Proteins Help DNA Replicate Past a Damaged Site” by the Oak Ridge Leadership Computing Facility.
12. Coverage of a publication in Nucleic Acids Research (2013), doi:10.1093/nar/gks1332. Featured science highlight “Neutrons help shed light on critical protein activity that protects our DNA” by ORNL’s Neutron Sciences Directorate.
13. Coverage of a publication in the Journal of the American Chemical Society (2010), doi:10.1021/ja100365x. Featured science highlight “Supercomputers Simulate the Molecular Machines that Replicate and Repair DNA” by the Oak Ridge Leadership Computing Facility.

SELECT INVITED PRESENTATIONS

1. Integrative modeling of the transcription-coupled repair molecular machinery. Computational Chemistry Gordon Research Conference, Castelldefels (Barcelona), Spain 2026
2. Molecular model of TFIIH recruitment to the transcription-coupled repair machinery. Seventh Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer, Cancun, Mexico 2026
3. Molecular model of TFIIH recruitment to the transcription-coupled repair machinery. Department of Biochemistry, Emory University, Atlanta, GA 2025
4. Molecular architecture and functional dynamics of the pre-incision complex in nucleotide excision repair. American Biophysical Society Thematic Meeting: Emerging Theoretical Approaches to Complement Single-Particle Cryo-Electron Microscopy, Trieste, Italy 2024
5. Dynamic conformational switching underlies TFIIH function in transcription and DNA repair and impacts genetic diseases. CECAM flagship workshop: Macromolecular complexes from ab initio and integrative modelling to functional dynamics, Lausanne, Switzerland 2023
6. Exascale supercomputing opens new avenues to model large biomolecular assemblies and uncover fundamental gene expression mechanisms. CECAM flagship workshop: Biomolecular simulation and machine learning in the exascale era, Pisa, Italy 2023
7. Dynamic conformational switching underlies TFIIH function in transcription and DNA repair and impacts genetic diseases. Annual Meeting of the American Society for Biochemistry and Molecular Biology (ASBMB), Seattle, WA 2023
8. Advanced computational modeling of molecular machines in transcription initiation. Biodesign Institute and Center for Biological Physics, Arizona State University, Tempe, AZ 2022
9. Advanced computational modeling of molecular machines in transcription initiation and DNA repair. Molecular Simulation 2020: Past, Present and Future, Erice, Italy 2022
10. Molecular simulation sheds light on the mechanisms of transcription-coupled DNA repair. Fifth Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer, Cancun, Mexico 2022
11. Molecular simulation sheds light on the mechanisms of transcription-coupled DNA repair. Biophysical and Biochemical Dynamics and Diffusion Symposium in Honor of J. Andrew McCammon, National Meeting of the American Chemical Society, San Diego, CA 2022
12. Advanced computational modeling of molecular machines in transcription initiation. Department of Medicinal Chemistry, Ohio State University, Columbus, OH 2022
13. Advanced computational modeling of molecular machines in transcription initiation. Department of Biochemistry & Molecular Biology, McGovern Medical School, University of Texas Health, Houston, TX 2021
14. Mechanism of Rad26-assisted rescue of stalled RNA polymerase II in transcription-coupled repair. 3rd Conference on Bio-motors, Virus Assembly, and RNA Nanobiotechnology, Ohio State University, Columbus, OH 2021
15. Advanced computational modeling of molecular machines in transcription initiation. Chemistry Department Seminar Program, Georgia State University, Atlanta, GA 2021

16. Advanced computational modeling of the molecular machines responsible for transcription initiation and nucleotide excision repair. Cellular and Molecular Biophysics (CMB) cluster of the Gulf Coast Consortium (GCC), Houston, TX 2021
17. Emerging unified description of transcription initiation from cryo-EM and integrative computational modeling. Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy 2021
18. Emerging unified description of transcription initiation from cryo-EM and integrative computational modeling. Fourth Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer, Nassau, Bahamas 2020
19. DNA sculpting as a strategy for base extrusion and damage selection by the repair glycosylase TDG. Lawrence Berkeley National Laboratory, Berkeley, CA 2018
20. Lesion search and base extrusion strategy of thymine DNA glycosylase. Third Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer, Cancun, Mexico 2018
21. Modeling biological assemblies from low to near atomic resolution. Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands 2016
22. Secondary Interaction Interfaces with PCNA Control Conformational Switching of DNA Polymerase PolB from Polymerization to Editing. Second Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer, Cancun, Mexico 2016
23. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct DNA damage response pathways. Department of Chemistry, Vanderbilt University, Nashville, TN 2014
24. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct DNA damage response pathways. Lawrence Berkeley National Laboratory, Berkeley, CA 2014
25. Integrative modeling of complex biological assemblies in DNA replication and transcription-coupled repair. Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer, Cancun, Mexico 2014
26. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct functional outcomes in the DNA damage response. Department of Biochemistry, Emory University School of Medicine, Atlanta, GA 2013
27. Proliferating cell nuclear antigen and its protein partners in DNA repair. Department of Biomolecular Sciences, University of Mississippi, Oxford, MS 2012
28. Integrative modeling of protein/DNA complexes at the replication fork. Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Minneapolis, MN 2012
29. Integrative modeling of FEN1 complexes with the sliding clamps PCNA and Rad9-Hus1-Rad1. Mutagenesis Gordon Research Conference, Newport, RI 2012
30. Solution phase X-ray scattering and multiscale computational modeling reveal the structural dynamics of ubiquitinated PCNA. Symposium in Honor of J. Andrew McCammon, 243rd National Meeting of the American Chemical Society, San Diego, CA 2012
31. Integrative modeling of protein/DNA complexes at the replication fork. Department of Molecular Biology and Biochemistry, Wesleyan University, Middletown, CT 2011
32. Integrative modeling of protein/DNA complexes at the replication fork. Conference on Computational Physics (CCP2011) 2011
33. Specific recognition of the ring-opened state of proliferating cell nuclear antigen by replication factor C promotes eukaryotic clamp-loading. Center for Molecular Biophysics, Oak Ridge National Laboratory, Oak Ridge, TN 2009
34. Specific recognition of the ring-opened state of proliferating cell nuclear antigen by replication factor C promotes eukaryotic clamp-loading. Frontiers in Macromolecular Simulations Symposium, Georgia Institute of Technology, Atlanta, GA 2009
35. The interplay of AAA+ molecular machines and sliding clamps at the DNA replication fork. Colorado Initiative in Molecular Biotechnology, University of Colorado, Boulder, CO 2009

36. The interplay of AAA+ molecular machines and sliding clamps at the DNA replication fork. Department of Chemistry, University of California Los Angeles, Los Angeles, CA 2009
37. Insight into DNA repair systems from classical and ab initio molecular dynamics. Department of Biophysics and Biophysical Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD 2007
38. Insight into DNA repair systems from classical and ab initio molecular dynamics. Department of Chemistry, Columbia University, New York, NY 2007
39. DNA repair systems and ligand-gated ion channels: Insights from classical and ab initio molecular dynamics. Department of Biochemistry, Washington University School of Medicine, St. Louis, MO 2007

CONTRIBUTED PRESENTATIONS (SELECTED FROM >70 PRESENTATIONS)

1. Molecular model of TFIIH recruitment to the transcription-coupled repair machinery. Cold Spring Harbor Laboratory Meeting: Mechanisms of Eukaryotic Transcription, Cold Spring Harbor, NY 2025
2. Molecular model of TFIIH recruitment to the transcription-coupled repair machinery. Federation of American Societies for Experimental Biology (FASEB) Meeting: Machines on Genes, Nashville, TN 2025
3. Molecular architecture and functional dynamics of the pre-incision complex in nucleotide excision repair. 268th National Meeting of the American Chemical Society, Denver, CO 2024
4. Structural and dynamic determinants of Rad26-mediated DNA damage discrimination by RNA Polymerase II. Pacifichem 2021 – International Chemical Congress of the Pacific Basin Societies, Honolulu, Hawaii (delivered online), 2021
5. Emerging unified description of transcription initiation from cryo-EM and integrative computational modeling. Pacifichem 2021 – International Chemical Congress of the Pacific Basin Societies, Honolulu, Hawaii (delivered online), 2021
6. Advanced computational modeling of molecular machines in transcription initiation. 262nd National Meeting of the American Chemical Society, Atlanta, GA 2021
7. Transcription initiation machinery functional dynamics and genetic disease. 257th National Meeting of the American Chemical Society, Orlando, FL 2019
8. Emerging unified description of transcription initiation from cryo-EM and integrative computational modeling. 256th National Meeting of the American Chemical Society, Boston, MA 2018
9. Electron microscopy and integrative modeling shed light on the structures of transcription pre-initiation complexes and the mechanisms of transcription initiation. Cryo-EM from Cells to Molecules: Multi-Scale Visualization of Biological Systems, Keystone Symposium, Tahoe City, CA 2018
10. Electron microscopy and integrative modeling shed light on the structures of transcription pre-initiation complexes and the mechanisms of transcription initiation. Nucleic Acids Gordon Research Conference, Biddeford, ME 2017
11. Integrative modeling of macromolecular assemblies in gene regulation. 5th Zing Nucleic Acids Conference, Tampa, FL 2016
12. Integrative modeling of macromolecular assemblies in gene regulation. Molecular Machines: Integrative Structural and Molecular Biology EMBO Conference, EMBL Heidelberg, Germany 2016
13. Damage recognition and base extrusion strategies of DNA repair glycosylase enzymes. 251st National Meeting of the American Chemical Society, San Diego, CA 2016
14. Hybrid modeling of ubiquitin- and SUMO-modified PCNA complexes: Implications for DNA damage responses. 251st National Meeting of the American Chemical Society, San Diego, CA 2016
15. Structurally distinct ubiquitin- and SUMO-modified PCNA: Implications for their distinct roles in the DNA damage response. Albany 2015 Conference, Albany, NY 2015
16. Integrative modeling of ubiquitinated and SUMOylated PCNA complexes. 4th Zing Nucleic Acids Conference, Cancun, Mexico 2014
17. Integrative modeling of protein assemblies involved in transcription. Biopolymers Gordon Research Conference, Newport, RI 2014

18. Integrative modeling of ubiquitinated and SUMOylated PCNA complexes. Annual Meeting of the Biophysical Society, San Francisco, CA 2014
19. Integrative modeling of complex biological assemblies in DNA replication and transcription-coupled repair. 246th National Meeting of the American Chemical Society, Indianapolis, IN 2013
20. Integrative modeling of ubiquitinated and SUMOylated PCNA complexes. Nucleic Acids Gordon Research Conference, Biddeford, ME 2013
21. Hybrid modeling of the ternary complexes of flap endonuclease-1 with sliding clamps and DNA. Keystone Meeting on Structural Analysis of Supramolecular Assemblies by Hybrid Methods, Tahoe City, CA 2013
22. Electron microscopy and computational modeling reveal key structural aspects of the ternary assemblies of flap endonuclease 1 with sliding clamps and DNA. 243rd National Meeting of the American Chemical Society, San Diego, CA 2012
23. Integrative modeling of protein/DNA complexes at the replication fork. 243rd National Meeting of the American Chemical Society, San Diego, CA 2012
24. Solution X-ray scattering reveals multiple modes of association for covalently bound ubiquitin on PCNA. Eukaryotic DNA Replication & Genome Maintenance meeting, Cold Spring Harbor Laboratory, NY 2011

AD HOC REVIEWER

Nature, Science, Chemical Reviews, Nature Structural & Molecular Biology, Nature Communications, Proceedings of the National Academy of Sciences USA, Journal of the American Chemical Society, Nucleic Acids Research, Accounts of Chemical Research, Journal of Physical Chemistry, ChemPhysChem, Journal of Chemical Theory and Computation, Biophysical Journal, Biochemistry, Chemical Communications, Journal of Chemical Physics, PLoS Computational Biology, PLoS One, Medicinal Research Reviews, Journal of Molecular Graphics and Modelling, Chemical Biology & Drug Design, Journal of Structural Biology, Journal of Chemical Information and Modeling, Journal of Physical Chemistry Letters, Frontiers in Molecular Biosciences.

RECENT COLLABORATIONS

Eva Nogales (Berkeley/HHMI); Yuan He (Johns Hopkins University); Stephen J. Benkovic (Pennsylvania State University); Y. George Zheng (University of Georgia); Eric Ortlund (Emory); Samir Hamdan (KAUST); Susan Tsutakawa (Lawrence Berkeley National Laboratory); John A. Tainer (M.D. Anderson Cancer Center); Dong Wang (UCSD); Huilin Li (Van Andel Institute); Alfredo de Biasio (KAUST).

SOCIETY MEMBERSHIPS

American Chemical Society (since 1999)
 Biophysical Society (since 2004)
 Protein Society (since 2004)
 Sigma Xi (Full membership since 2004)

TEACHING

Courses Taught

1. Physical Chemistry II (2010–2018; advanced undergraduate/graduate level)
2. Quantum Chemistry (2019–2025; advanced undergraduate/graduate level; developed an online version of this course and taught it in 2020 and 2021)
3. Physical Chemistry I (2010–2018; advanced undergraduate/graduate level)
4. Thermodynamics and Chemical Kinetics (2019–2020, 2024; advanced undergraduate/graduate level)
5. Instrumental Methods in Spectroscopy (2010–2015; advanced undergraduate laboratory)

6. Biophysical Chemistry (2012–2020; graduate level; team-taught with other biophysical division faculty)
7. Seminars in Chemistry (2011–2016; advanced undergraduate/graduate level; formal course based on the Chemistry Department seminar program)
8. Directed Research in Chemistry (2010–2025)
9. Undergraduate Research in Chemistry (2010–2025)

TRAINING AND MENTORING

Research Scientist

Dr. Chunli Yan (current)

Postdoctoral Scholars

Dr. Krishnendu Sinha (current)

Dr. Satyajit Khatua (current)

Dr. Sunil Tripathi (current)

Dr. Leonardo Serafim (current)

Dr. Tanmoy Paul (subsequently a position in industry, India)

Dr. Ashutosh Shandilya

Dr. Shashi Kumar (Asst. Professor, National Institute of Technology Rourkela, India)

Dr. Dheeraj Prakashchand (Asst. Professor, Indian Institute of Technology Mandi, India)

Dr. Jina Yu (Ph.D. from the group; continued briefly as a postdoctoral scholar, subsequently at Georgia Gwinnett College)

Dr. Thomas Dodd (Ph.D. from the group; continued for a year as a postdoctoral scholar, subsequently a data-science position in industry)

Dr. Kathleen Carter (Ph.D. from the group; continued briefly as a postdoctoral scholar, then Research Scientist at Emory University)

Dr. Buddhadev Maiti (subsequently postdoc at Carnegie Mellon University)

Dr. Carlo Guardiani (subsequently at the University of Warwick, UK)

Graduate Students

Kritika Varshney (current)

Emmanuel Bofo (current)

Dr. Jina Yu (Ph.D. awarded, subsequently at Georgia Gwinnett College)

Dr. Thomas Dodd (Ph.D. awarded, subsequently a data-science position in industry)

Dr. Kathleen Carter (Ph.D. awarded; continued briefly as a postdoctoral scholar in the group, then Research Scientist at Emory University)

Dr. Bradley Kossmann (Ph.D. awarded, subsequently Director of Data Science at Softcrylic Co.)

Dr. Xiaojun Xu (Ph.D. awarded, subsequently ORISE Fellow at the CDC and Senior Scientist at Pfizer)

Zhenyu Wang (M.S. awarded, subsequently an industry position in China)

Bernard Scott (M.S. awarded, subsequently Ph.D. at the University of Utah)

Shih-Wei Chuo (M.S. awarded, subsequently completed Ph.D. at the University of California, Davis)

Stephanie Kofsky (M.S. awarded, subsequently at Kemira Co.)

Patrick Chepaitis (M.S. awarded, subsequently scientist at GBI)

Yang Zhen (M.S. awarded)

Undergraduate Research Advisees

Fernando Cortez (2010), Amanuel Gebremariam (2011–2012), Oladayo Agboola (2011–2012), Bao-Khanh Ho (2011), Syiedah Korre (2011), Yosef Mekuria (2012), Evan Sinyard (2013), Albertha Sabree (2014), Eric Zientowski (2014), Zachary Ferris (2014), Annie Yoon (2015), Thomas Dodd (2015–2016), Lily Vassileva

(2016–2017), Nicole Ogbomoh (2016), Sam Delmerico (2017), Maia Wells (2017–2018), Kurt Martin, Grant Derdeyn-Blackwell (2022), Lucas Brewer (2023), Sofia Zeykan (2025–2026).

Student Awards

1. Molecular Basis of Disease Doctoral Fellowship: Xiaojun Xu, Kurt Martin, Tom Dodd, Bradley Kossmann
2. Molecular Basis of Disease Travel Fellowship: Bradley Kossmann
3. Dean's Doctoral Fellowship: Kathleen Carter
4. National Extreme Science and Engineering Discovery Environment Scholarship: Bernard Scott
5. Award for Outstanding Research at the Ph.D. level: Bradley Kossmann
6. Molecular Basis of Disease Outstanding Fellow Award: Bradley Kossmann, Tom Dodd
7. Hopkins Endowed Fellowship in Biophysical Chemistry: Tom Dodd, Jina Yu
8. Molecular Basis of Disease Undergraduate Fellowship: Grant Derdeyn-Blackwell

SERVICE (SELECTED)

2024	External Ph.D. examiner, King Abdullah University of Science and Technology, Saudi Arabia
2024	Guest editor, Proceedings of the National Academy of Sciences, USA
2023	Faculty Search Committee
2023	Chaired a session at the ASBMB 2023 meeting in Seattle, WA
2022	Panel reviewer for the MSFC Study Section, National Institutes of Health/CSR
2022	Organizer, ASBMB 2023 meeting in Seattle, WA
2022	Faculty Search Committee
2022	Panel reviewer for European Research Council (ERC) grants
2022	Panel reviewer for the MSFA Study Section, National Institutes of Health/CSR
2020 – 2025	Member, College of Arts & Sciences Promotion & Tenure Committee
2017 – Present	XSEDE (now ACCESS) Resource Allocation Committee (XRAC)
2017	Committee on Proposal Evaluation for Allocation of Supercomputing Time on the Special Purpose Anton Machine by D.E. Shaw Research
2017 – Present	European Science Foundation (ESF) College of Expert Reviewers
2016	Ad hoc reviewer for the National Institutes of Health/CSR
2016 – Present	Reviewing Editor, Frontiers Journals in Physics, Physiology and Molecular Biosciences
2015 – 2017	Member of the University Senate (Admissions & Standards; Planning & Development Committees), Georgia State University, Atlanta, GA
2013 – Present	Reviewer for regular NSF and NSF-CAREER proposals submitted to the MCB division of the National Science Foundation (Genetic Mechanisms Cluster)
2011 – 2016	Coordinator for the Chemistry Department seminar series