

CURRICULUM VITAE

Ivaylo Ivanov

Professor of Chemistry
Department of Chemistry, Georgia State University
P.O. Box 3965, Atlanta, GA 30302-3965
Email: iivanov@gsu.edu

A. EDUCATION

Ph.D. in Chemistry (2004)
Department of Chemistry, **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)
Department of Chemistry, **Carnegie Mellon University, Pittsburgh, PA**

B.S. in Chemistry (1996)
Department of Chemistry, **Sofia University, Sofia, Bulgaria**

B. PROFESSIONAL APPOINTMENTS

2020 - Present	Professor, Georgia State University, Atlanta, Georgia
2015 - 2020	Associate Professor, Georgia State University, Atlanta, Georgia
2009 - 2015	Assistant Professor, Georgia State University, Atlanta, Georgia
2012 - Present	Faculty, Center for Diagnostics & Therapeutics
2009 - Present	Faculty, Molecular Basis of Disease Program
2009 - Present	Faculty, Center for Biotechnology and Drug Design
2005 - 2009	Postdoctoral Research Associate, Department of Chemistry & Biochemistry, University of California-San Diego, La Jolla, CA

C. RESEARCH

C.1 Publications (72 publications, cited >4500 times in Google Scholar, h-index 40)

1. Syed A., Serafim, L. F., Arvai, A. S., Tang, H. Y. H, Huffman, J. L., Mol, C. D., Hitomi, K., Parikh, S., Tsai, S. L., Bacolla, A., Shin, D. S., Cunningham, R. P., Iwai, S., Chowdhury, D., **Ivanov, I.*** & Tainer, J.A.* Unified catalytic mechanism for purine/pyrimidine glycosylase-1 AP-lyase oxidized DNA base removal. (Under review in *Nature Communications*)
2. Kim, M., Jeong, E., Park, J., Tsai, M-S., Yan, C., **Ivanov, I.**, Kim, S.K., Schärer O. D., The interaction of XPG with TFIIH through p62 and XPD is required for the completion of nucleotide excision repair. (Under review in *Nucleic Acids Research*), BioRxiv doi: 10.1101/2025.05.20.655039
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), doi:10.1038/s41467-025-66834-1, PMID: 41315283.

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, PMCID: 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, PMCID: 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, PMCID: 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, PMCID: 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., Mosammaparast, 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, PMCID: 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, PMCID: 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, PMCID: 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, PMCID: 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, PMCID: 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, PMCID: PMC8130551.
15. Tsutakawa, S. E., Tsai, C. L., Yan, C., Bralic, A., Chazin, W. J., Hamdan, S. M., Scharer, 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, PMCID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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, PMID: 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.
30. He, Y., Yan, C., Fang, J., Inouye, C., Tjian, R., **Ivanov, I.** & Nogales, E. Near-atomic resolution visualization of human transcription promoter opening. *Nature* (2016) **533**, 359, doi:10.1038/nature17970, PMCID: PMC4940141. **(highlighted by the Texas Advanced Computing Center; cited >300 times)**
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.jpcb.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., Wohlueter, 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.
35. Brosey, C. A., Soss, S. E., Brooks, S., Yan, C., **Ivanov, I.**, Dorai, K. & Chazin, W. J. Functional dynamics in replication protein A DNA binding and protein recruitment domains. *Structure* (2015) **23**, 1028, doi:10.1016/j.str.2015.04.008, PMCID: PMC4456234.
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.
37. Kossmann, B. & **Ivanov, I.*** Alkylpurine glycosylase D employs DNA sculpting as a strategy to extrude and excise damaged bases. *PLoS Computational Biology* (2014) **10**, e1003704, doi:10.1371/journal.pcbi.1003704, PMCID: PMC4081403.
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.
40. Wang, L., Xu, X., Kumar, R., Maiti, B., Liu, C. T., **Ivanov, I.***, Lee, T. H. & Benkovic, S. J. Probing DNA clamps with single-molecule force spectroscopy. *Nucleic Acids Research* (2013) **41**, 7804, doi:10.1093/nar/gkt487, PMCID: PMC3763527.
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/aprimidinic 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)**
42. Brosey, C. A., Yan, C., Tsutakawa, S. E., Heller, W. T., Rambo, R. P., Tainer, J. A., **Ivanov, I.*** & Chazin, W. J. A new structural framework for integrating replication protein A into DNA processing machinery. *Nucleic Acids Research* (2013) **41**, 2313, doi:10.1093/nar/gks1332, PMCID: PMC3575853. **(selected as a featured paper in the top 5% of NAR submissions)**

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**)
47. Feng, Y., Wang, J., Asher, S., Hoang, L., Guardiani, C., **Ivanov, I.*** & Zheng, Y. G. Histone H4 acetylation differentially modulates arginine methylation by an in cis mechanism. *Journal of Biological Chemistry* (2011) **286**, 20323, doi:10.1074/jbc.M110.207258, PMCID: PMC3121530. (**recommended by Faculty of 1000 Prime; cited >100 times**)
48. Sander, T., Frolund, B., Bruun, A. T., **Ivanov, I.**, McCammon, J. A. & Balle, T. New insights into the GABA(a) receptor structure and orthosteric ligand binding: Receptor modeling guided by experimental data. *Proteins* (2011) **79**, 1458, doi:10.1002/prot.22975, PMCID: PMC3076690.
49. Fritsch, S., **Ivanov, I.**, Wang, H. & Cheng, X. Ion selectivity mechanism in a bacterial pentameric ligand-gated ion channel. *Biophysical Journal* (2011) **100**, 390, doi:10.1016/j.bpj.2010.11.077, PMCID: PMC3021669.
50. Tainer, J. A., McCammon, J. A. & **Ivanov, I.*** Recognition of the ring-opened state of proliferating cell nuclear antigen by replication factor C promotes eukaryotic clamp-loading. *Journal of the American Chemical Society* (2010) **132**, 7372, doi:10.1021/ja100365x, PMCID: PMC2876781. (**highlighted by the National Center for Computational Sciences**)
51. Cheng, X., **Ivanov, I.**, Wang, H., Sine, S. M. & McCammon, J. A. Molecular dynamics simulations of ELIC - a prokaryotic homologue of the nicotinic acetylcholine receptor. *Biophysical Journal* (2009) **96**, 4502, doi:10.1016/j.bpj.2009.03.018, PMCID: PMC2711484.
52. Amaro, R. E., Cheng, X., **Ivanov, I.**, Xu, D. & McCammon, J. A. Characterizing loop dynamics and ligand recognition in human- and avian-type influenza neuraminidases via Generalized Born molecular dynamics and end-point free energy calculations. *Journal of the American Chemical Society* (2009) **131**, 4702, doi:10.1021/ja8085643, PMCID: PMC2665887. (**cited >150 times**)
53. Som, A., Vemparala, S., **Ivanov, I.** & Tew, G. N. Synthetic mimics of antimicrobial peptides. *Biopolymers* (2008) **90**, 83, doi:10.1002/bip.20970, PMID: 18314892. (**cited >200 times**)
54. Gorfe, A. A., Chang, C. E., **Ivanov, I.** & McCammon, J. A. Dynamics of the acetylcholinesterase tetramer. *Biophysical Journal* (2008) **94**, 1144, doi:10.1529/biophysj.107.117879, PMCID: PMC2212707.
55. Cheng, X., **Ivanov, I.***, Wang, H., Sine, S. M. & McCammon, J. A. Nanosecond-timescale conformational dynamics of the human alpha7 nicotinic acetylcholine receptor. *Biophysical Journal* (2007) **93**, 2622, doi:10.1529/biophysj.107.109843, PMCID: PMC1989720.
56. **Ivanov, I.***, Cheng, X., Sine, S. M. & McCammon, J. A. Barriers to ion translocation in cationic and anionic receptors from the cys-loop family. *Journal of the American Chemical Society* (2007) **129**, 8217, doi:10.1021/ja070778l, PMID: 17552523.
57. **Ivanov, I.***, Tainer, J. A. & McCammon, J. A. Unraveling the three-metal-ion catalytic mechanism of the DNA repair enzyme endonuclease IV. *Proceedings of the National Academy of Sciences USA* (2007) **104**, 1465, doi:10.1073/pnas.0603468104, PMCID: PMC1780068. (**cited >100 times**)

58. **Ivanov, I.***, Chapados, B. R., McCammon, J. A. & Tainer, J. A. Proliferating cell nuclear antigen loaded onto double-stranded DNA: Dynamics, minor groove interactions and functional implications. *Nucleic Acids Research* (2006) **34**, 6023, doi:10.1093/nar/gkl744, PMCID: PMC1635319. (**cited >100 times**)
59. Vemparala, S., **Ivanov, I.**, Pophristic, V., Spiegel, K. & Klein, M. L. Ab initio calculations of intramolecular parameters for a class of arylamide polymers. *J Comput Chem* (2006) **27**, 693, doi:10.1002/jcc.20382, PMID: 16634095.
60. **Ivanov, I.***, Chen, B., Raugei, S. & Klein, M. L. Relative pKa values from first-principles molecular dynamics: The case of histidine deprotonation. *Journal of Physical Chemistry B* (2006) **110**, 6365, doi:10.1021/jp056750i, PMID: 16553455.
61. Pophristic, V., Vemparala, S., **Ivanov, I.**, Liu, Z., Klein, M. L. & DeGrado, W. F. Controlling the shape and flexibility of arylamides: A combined ab initio, ab initio molecular dynamics, and classical molecular dynamics study. *Journal of Physical Chemistry B* (2006) **110**, 3517, doi:10.1021/jp054306+, PMID: 16494407.
62. **Ivanov, I.***, Vemparala, S., Pophristic, V., Kuroda, K., DeGrado, W. F., McCammon, J. A. & Klein, M. L. Characterization of nonbiological antimicrobial polymers in aqueous solution and at water-lipid interfaces from all-atom molecular dynamics. *Journal of the American Chemical Society* (2006) **128**, 1778, doi:10.1021/ja0564665, PMID: 16464062. (**Faculty of 1000 Prime recommended; cited >100 times**)
63. Choi, S., Clements, D. J., Pophristic, V., **Ivanov, I.**, Vemparala, S., Bennett, J. S., Klein, M. L., Winkler, J. D. & DeGrado, W. F. The design and evaluation of heparin-binding foldamers. *Angewandte Chemie-International Edition* (2005) **44**, 6685, doi:10.1002/anie.200501279, PMID: 16094685. (**featured on the cover of Angewandte Chemie; cited >100 times**)
64. **Ivanov, I.*** & Klein, M. L. Dynamical flexibility and proton transfer in the arginase active site probed by ab initio molecular dynamics. *Journal of the American Chemical Society* (2005) **127**, 4010, doi:10.1021/ja043693i, PMID: 15771538.
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66. **Ivanov, I.** Terascale ab initio molecular dynamics simulations of proton transfer and dissociation processes in chemical and biological systems. University of Pennsylvania (2004) ProQuest, 305143649.
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68. Chen, B., **Ivanov, I.**, Klein, M. L. & Parrinello, M. Hydrogen bonding in water. *Physical Review Letters* (2003) **91**, 215503, doi:10.1103/PhysRevLett.91.215503, PMID: 14683314. (**cited >400 times**)
69. Min, G., Savin, D., Gu, Z., Patterson, G. D., Kim, S. H., Ramsay, D. J., Fishman, D., **Ivanov, I.**, Sheina, E., Slaby, E., Oliver, J. Solution characterization of monodisperse atactic polystyrenes by static and dynamic light scattering. *International Journal of Polymer Analysis and Characterization* (2003) **8**, 187-207, doi:10.1080/10236660304875.
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* denotes corresponding author

C.2 Grants and Awards

C.2.1 Research Funding

1. National Institute of Environmental Health Sciences R01 ES032786 (4/1/22 – 3/31/27); Title: “Integrative Modeling of Biomolecular Machinery in Nucleotide Excision Repair”; Role: Principal Investigator; Total cost: **\$2,082,459**
2. 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**
3. 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**
4. 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**
5. 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**
6. 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**
7. 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**
8. 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.)
9. 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**
10. 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.)
11. 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**

C.2.2 Computational Support at the National Supercomputing Facilities (selected awards)

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. Innovative and Novel Computational Impact on Theory and Experiment (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. Innovative and Novel Computational Impact on Theory and Experiment (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. Innovative and Novel Computational Impact on Theory and Experiment (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. Innovative and Novel Computational Impact on Theory and Experiment (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. Innovative and Novel Computational Impact on Theory and Experiment (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. Innovative and Novel Computational Impact on Theory and Experiment (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. Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award (1/1/2019 – 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. Innovative and Novel Computational Impact on Theory and Experiment (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.

C.2.3 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)

C.3 Recognition and Media Coverage

1. Coverage of a publication in *Nature Communications* (2025),
doi:10.1038/s41467-025-57593-0
Altmetric score 36. This article is in the **95th percentile** (ranked 7,543rd) of the 170,252 tracked articles of a similar age in all journals and the **85th percentile** (ranked 205th) of the 1,427 tracked articles of a similar age in *Nature Communications*. Featured on the website of the Oak Ridge Leadership Computing Facility in a news story "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. This article is in the **97th percentile** (ranked 9,419th) of the 316,219 tracked articles of a similar age in all journals and the **85th percentile** (ranked 340th) of the 2,424 tracked articles of a similar age in *Nature Communications*. Featured on the website of the Oak Ridge Leadership Computing Facility in a news story "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. This article is in the **92nd percentile** (ranked 27,860) of the 375,925 tracked articles of a similar age in all journals and the **68th percentile** (ranked 631) of the 2,034 tracked articles of a similar age in *Nature Communications*. Featured on the website of the Oak Ridge Leadership Computing Facility in a news story "New Insights into a Shapeshifting Protein Complex".
4. Coverage of a publication in *Nature Communications* (2021),
doi:10.1038/s41467-021-27295-4
Featured on the website of the Oak Ridge Leadership Computing Facility in a news story "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. This article is in the **87th percentile** (ranked 53,523) of the 419,570 tracked articles of a similar age in all journals and the **46th percentile** (ranked 918) of the 1,710 tracked articles of a similar age in *Nature Communications*. Featured on the website of the Oak Ridge Leadership Computing Facility in a news story "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. The article is in the **96th percentile** (ranked 4,371) of the 118,590 tracked articles of a similar age in all journals and in the **85th percentile** (ranked 2) of the 14 tracked articles of a similar age in *Nature Structural & Molecular Biology*. Featured on the website of the Oak Ridge Leadership Computing Facility in a news story “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 on the website of the San Diego Supercomputer Center in a news story “How an Enzyme Repairs DNA via a Pinch-Push-Pull Mechanism”. Highlighted by the following news outlets: *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. The article is in the **98th percentile** (ranked 3,654) of the 227,366 tracked articles of a similar age in all journals and in the **60th percentile** (ranked 388) of the 975 tracked articles of a similar age in *Nature*. Highlighted by the *Science360* site and the MCB Division of the National Science Foundation, *Phys.org*, *Technology.org*, *e!Science News*, *Nanowerk*, *Bioportfolio*, *EurekAlert!*, *Newswise* and *Science Daily* among other media sources. Highlighted by the Texas Advanced Computing Center in a news story “How to See Living Machines”.

9. Coverage of a publication in *Nature Communications* (2016), doi:10.1038/ncomms11675

Altmetric score 201. The article is in the **99th percentile** (ranked 1,781) of the 190,421 tracked articles of a similar age in all journals and in the **94th percentile** (ranked 37) of the 713 tracked articles of a similar age 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. The article is in the **96th percentile** of the 252241 tracked articles of a similar age in all journals and in the **76th percentile** (ranked 238) of the 1024 tracked articles of a similar age in *PNAS*. Highlighted by *ScienceDaily*, *Health Medicine Network*, *PhysOrg.com* and *EurekAlert!* among other media sources.

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 (OLCF) at Oak Ridge National Laboratory (<https://www.olcf.ornl.gov/2011/11/09>).

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 the ORNL's Neutron Sciences Directorate, Oak Ridge National Laboratory (<http://neutrons2.ornl.gov/research/highlights/BioSANS/protein-activity-dna.html>).

13. Coverage of a publication in the *Journal of the American Chemical Society* (2010), doi:10.1021/ja100365x

Featured in a science highlight entitled “Supercomputers Simulate the Molecular Machines that Replicate and Repair DNA” by the Oak Ridge Leadership Computing Facility (OLCF) of Oak Ridge National Laboratory (<https://www.olcf.ornl.gov/2010/06/24/>).

C.4 Select Invited Presentations

1. Molecular model of TFIIH recruitment to the transcription-coupled repair machinery. *Seventh Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer*, Mexico 2026 (scheduled)

2. Molecular model of TFIIH recruitment to the transcription-coupled repair machinery. *Department of Biochemistry, Emory University, Atlanta, GA* 2025
3. 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
4. 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
5. 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: first applications and perspectives*. Pisa, Italy 2023
6. 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
7. Advanced computational modeling of molecular machines in transcription initiation., *Biodesign Institute and Center for Biological Physics, Arizona State University, Tempe, AZ* 2022
8. Advanced computational modeling of molecular machines in transcription initiation and DNA repair. *Molecular Simulation 2020: Past, Present and Future*, Erice, Italy 2022
9. Molecular simulation sheds light on the mechanisms of transcription-coupled DNA repair. *Fifth Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer*, Mexico 2022
10. 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
11. Advanced computational modeling of molecular machines in transcription initiation. *Department of Medicinal Chemistry, Ohio State University, Columbus, OH* 2022
12. Advanced computational modeling of molecular machines in transcription initiation. *Department of Biochemistry & Molecular Biology, McGovern Medical School, University of Texas Health*, Houston, TX 2021
13. 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
14. Advanced computational modeling of molecular machines in transcription initiation. *Chemistry Department Seminar Program, Georgia State University, Atlanta, GA* 2021
15. 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
16. Emerging unified description of transcription initiation from cryo-EM and integrative computational modeling. *Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy* 2021
17. 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
18. DNA sculpting as a strategy for base extrusion and damage selection by the repair glycosylase TDG. *Lawrence Berkeley National Laboratory, Berkeley, CA* 2018
19. Lesion search and base extrusion strategy of thymine DNA glycosylase. *Third Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer*, Cancun, Mexico 2018
20. Modeling biological assemblies from low to near atomic resolution. *Van't Hoff Institute for Molecular Sciences*,

University of Amsterdam, Amsterdam, The Netherlands 2016

21. 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
22. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct DNA damage response pathways. *Department of Chemistry, Vanderbilt University*, Nashville, TN 2014
23. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct DNA damage response pathways. *Lawrence Berkeley National Laboratory*, Berkeley, CA 2014
24. 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
25. 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
26. Proliferating cell nuclear antigen and its protein partners in DNA repair. *Department of Biomolecular Sciences, University of Mississippi*, Oxford, MS 2012
27. Integrative modeling of protein/DNA complexes at the replication fork. *Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota*, Minneapolis, MN 2012
28. Integrative modeling of FEN1 complexes with the sliding clamps PCNA and Rad9-Hus1-Rad1. *Mutagenesis Gordon Research Conference*, Newport, RI 2012
29. 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
30. Integrative modeling of protein/DNA complexes at the replication fork. *Department of Molecular Biology and Biochemistry, Wesleyan University*, Middletown, CT 2011
31. Integrative modeling of protein/DNA complexes at the replication fork. *Conference on Computational Physics (CCP2011)* 2011
32. 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
33. 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
34. 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
35. 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
36. 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
37. Insight into DNA repair systems from classical and ab initio molecular dynamics. *Department of Chemistry, Columbia University*, New York, NY 2007
38. 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

C.5 Contributed Presentations (selected out of >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. 270th *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. *Pacificchem 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, *Pacificchem 2021 – International Chemical Congress of the Pacific Basin Societies*, Honolulu, Hawaii (delivered online), 2021
6. Advanced computational modeling of molecular machines in transcription initiation. 264th *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 2018
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

C.6 Ad Hoc Reviewer

Nature, Science, Chemical Reviews, Nature Structural & Molecular Biology, Nature Communications, Proceedings of the National Academy of Science 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

C.7 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 (Berkeley National Laboratory)

John A. Tainer (M.D. Anderson Cancer Center)

Dong Wang (UCSD)

C.8 Society Memberships

American Chemical Society (since 1999)

Biophysical Society (since 2004)

Protein Society (since 2004)

Sigma Xi (Full membership since 2004)

D. TEACHING AND MENTORING**D.1 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)

D.2 Training and Mentoring

Research Scientist

Dr. Chunli Yan (current)

Postdoctoral Scholars

Dr. Krishnendu Singha (current)

Dr. Satyajit Khatua (current)

Dr. Tanmoy Paul (current)

Dr. Sunil Tripathi (current)

Dr. Leonardo Serafim (current)

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

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

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

Dr. Kathleen Carter (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)

Jina Yu (Ph.D. awarded)

Thomas Dodd (Ph.D. awarded, subsequently obtained data science industry position)

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

Dr. Kathleen Carter (Ph.D. awarded, subsequently Research Scientist at Emory University)

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

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)

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)

Undergraduates 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), Grant Derdeyn-Blackwell (2022), Lucas Brewer (2023)

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

E. SERVICE (selected contributions)

2024	External PhD examiner, King Abdullah University of Science and Technology, Saudi
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 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