

CURRICULUM VITAE

Ivaylo Ivanov

Professor of Chemistry
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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 (62 publications, cited 2980 times in Google Scholar, h-index 32)

1. 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. under review, *Nature Communications*
2. Dodd, T., Yao, X., Hamelberg, D. & **Ivanov, I.*** Subsets of adjacent nodes (SOAN): A fast method for computing suboptimal paths in protein dynamic networks. (2021) *Molecular Physics*, doi:10.1080/00268976.2021.1893847 (**Invited article for the Michael L. Klein special issue**)
3. Dodd, T., Botto, M., Paul, F., Leiro, R.F, Lamers, M.H., & **Ivanov, I.*** Defined path for conformational switching from polymerization to editing in a high-fidelity DNA polymerase. (2020) *Nature Communications* 11, 5379, doi:10.1038/s41467-020-19165-2 (**highlighted by the Oak Ridge Leadership Computing Facility**)
4. Tsutakawa, S.E., Tsai, C-L., Yan, C., Bralić, 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. (2020) *DNA Repair*, 96, 102972, doi:10.1016/j.dnarep.2020.102972
5. Qian, K., Yan, C., Su, H., Dang, T., Zhou, B., Wang, Z., Zhao, X., **Ivanov, I.** & Zheng, Y.G. Pharmacophore-based screening of diamidine small molecule inhibitors for protein arginine methyltransferases. *RCS Medicinal Chemistry* (2020), doi:10.1039/D0MD00259C
 6. Yuan, Z., Schneider, S., Dodd, T., Riera, A., Bai, L., Yan, C., **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, 17747-17756, doi:10.1073/pnas.2006231117
 7. Dodd, T., Yan, C., & **Ivanov, I.*** Simulation-based methods for model building and refinement in cryo-electron microscopy. *Journal of Chemical Information and Modeling* (2020) 60, 5, 2470–2483 doi:10.1021/acs.jcim.0c00087
 8. Yan, C., Dodd, T., Tainer, J.A., He, Y., Tsutakawa, S.E., & **Ivanov, I.*** Transcription preinitiation complex structure and dynamics provide insight into genetic diseases. *Nature Structural & Molecular Biology* (2019), 26, 397-406, doi:10.1038/s41594-019-0220-3 (**recommended by Faculty of 1000 Prime; highlighted by the Oak Ridge Leadership Computing Facility at <https://www.olcf.ornl.gov/2019/05/20/>**)
 9. 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 interfaces integrity in DNA clamps. *Journal of Molecular Biology* (2019), 431, 2493-2510, doi:10.1016/j.jmb.2019.04.035
 10. Carter, E.K., Laughlin-Toth, S., Dodd, T., Wilson, D.W. & **Ivanov, I.*** Small molecule binders recognize DNA microstructural variations via an induced fit mechanism. *Physical Chemistry Chemical Physics* (2019) 21, 1841-1851, doi:10.1039/C8CP05537H
 11. 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, 5974-5979, doi:10.1073/pnas.1803323115 (**highlighted by the San Diego Supercomputer Center**)
 12. Li, J., Li, S., Guo, J., Li, Q., Long, J., Ma, C., Ding, Y., Yan, C., Li, L., Wu, Z., Zhu, H., Li, K., Wen, L., Zhang, Q., Xue, Q., Zhao, C., Liu, N., **Ivanov, I.**, Luo, M., Xi, R., Long, H., Wang, P.W. & Chen, Y. Natural product Micheliolide (MCL) irreversibly activates pyruvate kinase M2 and suppresses leukemia. *Journal of Medicinal Chemistry* (2018) 61, 4155–4164, doi:10.1021/acs.jmedchem.8b00241
 13. 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
 14. Han, Y., Yan, C., Nguyen, K., Jackobel, A., **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
 15. Rashid F. et al. Single-molecule FRET unveils induced-fit mechanism for substrate selectivity in flap endonuclease 1. *eLife* (2017) 6, e21884, doi:10.7554/eLife.21884 (**recommended by Faculty of 1000 Prime**)
 16. Zhang, J., Qian, K., Yan, C., He, M., Jassim, B., **Ivanov, I.** & Zheng, Y. Discovery of decamidine as a new and potent PRMT1 inhibitor. *Medicinal Chemistry Communications* (2017) 8, 440-444, doi:10.1039/C6MD00573J
 17. Laughlin, 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, 1297-1306, doi:10.1093/nar/gkw1232
 18. He, Y., Yan, C., Inouye, C., Fang, J., Tjian, R., **Ivanov, I.** & Nogales E. Structural basis of transcription promoter opening using single particle cryo-EM. *Nature* (2016) 533, 359–365, doi:10.1038/nature17970 (**cited >200 times; highlighted by the Texas Advanced Computing Center**)
 19. Turaga, R.C., Yin, L., Yang, J.J., Lee, H., **Ivanov, I.**, Yan, C., Grossniklaus, H.E., Wang, S., Ma, C., Sun, L. & Liu, Z. Development of protein drug targeting integrin $\alpha\beta 3$ at a novel site by rational protein design. *Nature Communications* (2016) 7, 11675, doi:10.1038/ncomms11675

20. Hudson, W.H., Kossmann, B., de Vera, I.M., Chuo, S.W., Weikum, E.A., Eick G., Thornton, J., **Ivanov, I.**, Kojetin, D.J., & Ortlund, E.A. Distal substitutions drive divergent DNA specificity among paralogous transcription factors through a subdivision of conformational space. *Proceedings of the National Academy of Sciences USA* (2016) 113, 326-331, doi:10.1073/pnas.1518960113
21. Xu, X., Yan, C., Kossmann, B. & **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, 8379–8388, doi:10.1021/acs.jpcc.6b02082 (**Invited article for the J. Andrew McCammon Festschrift special issue**)
22. Kossmann, B., Marchand C, Pommier Y* & **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, 3232-3236, doi:10.1016/j.bmcl.2016.05.065
23. Musille, P. M., Kossmann, B., Kohn, J. A., **Ivanov, I.**, & Ortlund E. A. Unexpected allosteric network contributes to LRH-1 co-regulator selectivity. *Journal of Biological Chemistry* (2016) 291, 1411-1426, doi:10.1074/jbc.M115.662874
24. 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, 492–503, doi:10.1016/j.csbj.2015.08.005
25. Brosey, C.A., Soss, S.E., Brooks, S., Yan, C., **Ivanov, I.**, Dorai, K., & Chazin, W.J. Functional dynamics in RPA DNA binding and protein recruitment domains. *Structure* (2015) 23, 1028–1038, doi:10.1016/j.str.2015.04.008
26. Tsutakawa, S.E., Yan, C., Xu, X., Weinacht, C., Frudental, B., 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, 724–733, doi:10.1016/j.str.2015.02.008
27. 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
28. Yan, L., Yan, C., Su, H., Qian, K., Wofford, S., Zhao, X., **Ivanov, I.*** & Zheng Y.G. Diamidine compounds as selective inhibitors of protein arginine methyltransferase 1. *Journal of Medicinal Chemistry* (2014) 57, 2611–2622, doi:10.1021/jm401884z
29. 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, 10020-10031, doi:10.1093/nar/gkt810
30. 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, 7804-7814, doi:10.1093/nar/gkt487
31. 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, 8445-8455, doi:10.1074/jbc.M112.422774
32. **Ivanov, I.*** Enzyme cofactors: Double-edged sword for catalysis. *Nature Chemistry* (2013) 5, 6-7, doi:10.1038/nchem.1529
33. 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, 2313-2327, doi:10.1093/nar/gks1332 (**selected as a featured paper in the top 5% of NAR submissions**)
34. 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, 8528-8533, doi:10.1073/pnas.1121116109
35. Cheng, X. & **Ivanov, I.** Molecular dynamics. *Methods in Molecular Biology (Clifton, N.J.)* (2012) 929, 243-285 (Springer Protocols Series; ISBN 978-1-62703-049-6)
 36. 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, 17672-17677, doi:10.1073/pnas.1110480108 (**recommended by Faculty of 1000 Prime; highlighted by the Oak Ridge Leadership Computing Facility at <http://www.olcf.ornl.gov/2011/11/09>**)
 37. 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: Structure Function and Bioinformatics* (2011) 79, 1458-1477, doi:10.1002/prot.22975
 38. Fritsch, S., **Ivanov, I.**, Wang, H. & Cheng, X. Ion selectivity mechanism in a bacterial pentameric ligand-gated ion channel. *Biophysical Journal* (2011) 100, 390-398, doi:10.1016/j.bpj.2010.11.077
 39. 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, 20323-20334, doi:10.1074/jbc.M110.207258 (**recommended by Faculty of 1000 Prime**)
 40. 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, 7372-7378, doi:10.1021/ja100365x (**highlighted by the National Center for Computational Sciences (NCCS) at <http://www.nccs.gov/2010/06/24>**)
 41. 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, 4502-4513, doi:10.1016/j.bpj.2009.03.018
 42. 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, 4702-4709, doi:10.1021/ja8085643 (**cited >100 times**)
 43. Som, A., Vemparala, S., **Ivanov, I.** & Tew, G. N. Synthetic mimics of antimicrobial peptides. *Biopolymers* (2008) 90, 83-93, doi:10.1002/bip.20970 (**cited >150 times**)
 44. Gorfe, A. A., Chang, C. E. A., **Ivanov, I.** & McCammon, J. A. Dynamics of the acetylcholinesterase tetramer. *Biophysical Journal* (2008) 94, 1144-1154, doi:10.1529/biophysj.107.117879
 45. **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, 1465-1470, doi:10.1073/pnas.0603468104 (**cited >100 times**)
 46. **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, 8217-8224, doi:10.1021/ja070778l
 47. Cheng, X., **Ivanov, I.***, Wang, H., Sine, S. M. & McCammon, J. A. Nanosecond timescale conformational dynamics of the human alpha 7 nicotinic acetylcholine receptor. *Biophysical Journal* (2007) 93, 2622-2634, doi:10.1529/biophysj.107.109843
 48. Vemparala, S., **Ivanov, I.**, Pophristic, V., Spiegel, K. & Klein, M. L. Ab initio calculations of intramolecular parameters for a class of arylamide polymers. *Journal of Computational Chemistry* (2006) 27, 693-700, doi:10.1002/jcc.20382
 49. Pophristic, V., Vemparala, S., **Ivanov, I.**, Liu, Z. W., 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, 3517-3526, doi:10.1021/jp054306

50. **Ivanov, I.***, Vemparala, S., Pophristic, V., Kuroda, K., DeGrado, W. F., McCammon, J. A. & Klein, M. L. Characterization of non-biological antimicrobial polymers in aqueous solution and at water-lipid interfaces from all-atom molecular dynamics. *Journal of the American Chemical Society* (2006) 128, 1778-1779, doi:10.1021/ja0564665 (**Faculty of 1000 Prime recommended**)
51. **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, 6365-6371, doi:10.1021/jp056750i
52. **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, 6023-6033, doi:10.1093/nar/gkl744
53. **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, 4010-4020, doi:10.1021/ja043693i
54. Choi, S., Clements, D. J., Pophristic, V., **Ivanov, I.**, Vemparala, S., Bennett, J. S., Klein, M. L., Winkler, J. D. & DeGrado, W. E. The design and evaluation of heparin-binding foldamers. *Angewandte Chemie-International Edition* (2005) 44, 6685-6689, doi:10.1002/anie.200501279 (**featured on the cover of Angewandte Chemie**)
55. **Ivanov, I.** Terascale ab initio molecular dynamics simulations of proton transfer and dissociation processes in chemical and biological systems. (2004) *ProQuest* AAI3152059
56. Nielsen, S. O., Lopez, C. F., **Ivanov, I.**, Moore, P. B., Shelley, J. C. & Klein, M. L. Transmembrane peptide-induced lipid sorting and mechanism of L-alpha-to-inverted phase transition using coarse-grain molecular dynamics. *Biophysical Journal* (2004) 87, 2107-2115, doi:10.1529/biophysj.104.040311
57. **Ivanov, I.*** & Klein, M. L. First principles computational study of the active site of arginase. *Proteins: Structure Function and Genetics* (2004) 54, 1-7, doi:10.1002/prot.10572
58. 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
59. Chen, B., **Ivanov, I.**, Klein, M. L. & Parrinello, M. Hydrogen bonding in water. *Physical Review Letters* (2003) 91, doi:10.1103/PhysRevLett.91.215503 (**cited >350 times**)
60. **Ivanov, I.*** & Klein, M. L. Deprotonation of a histidine residue in aqueous solution using constrained ab initio molecular dynamics. *Journal of the American Chemical Society* (2002) 124, 13380-13381, doi:10.1021/ja027972m
61. Chen, B., Park, J. M., **Ivanov, I.**, Tabacchi, G., Klein, M. L. & Parrinello, M. First-principles study of aqueous hydroxide solutions. *Journal of the American Chemical Society* (2002) 124, 8534-8535, doi:10.1021/ja020350g
62. Chen, B., **Ivanov, I.**, Park, J. M., Parrinello, M. & Klein, M. L. Solvation structure and mobility mechanism of OH⁻: A Car-Parrinello molecular dynamics investigation of alkaline solutions. *Journal of Physical Chemistry B* (2002) 106, 12006-12016, doi:10.1021/jp026504w (**cited >100 times**)
63. **Ivanov, I.**, Gherman, B. F. & Yaron, D. Comparison of the INDO band structures of polyacetylene, polythiophene, polyfuran, and polypyrrole. *Synthetic Metals* (2001) 116, 111-114, doi:10.1016/s0379-6779(00)00526-9

* denotes corresponding author

C.2 Grants and Awards

C.2.1 Research Funding

1. National Institute of General Medical Sciences R35 GM139382 (3/1/21 – 2/28/26); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation and DNA Repair”; Role: Principal Investigator; Total cost: **\$2,261,126**
2. National Science Foundation MCB-2027902 (8/1/20 – 7/31/24); Title: “Advanced Computational Modeling of Pathways for Epigenetic Regulation and Genome Maintenance”; Role: Principal Investigator; Total cost: **\$765,882**
3. National Cancer Institute P01 CA092584 (9/27/21 – 8/31/26); Title: "Structural Cell Biology of DNA Repair Machines"; Role: Senior Investigator; Total cost: **\$424,780**
4. 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**
5. 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**
6. 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**
7. 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.)
8. 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**
9. 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.)
10. 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**
11. **Pending**: National Institute of Environmental Health Sciences R01 ES032786 (12/1/21 – 11/30/26); Title: “Integrative Modeling of Biomolecular Machinery in Nucleotide Excision Repair”; Role: Principal Investigator

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

1. Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award (1/1/21 – 12/31/21); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation”; Role: Principal Investigator; Awarded 260,000 service units (>25 million CPU hours and 3,000,000 GPU hours) 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 (1/1/20 – 12/31/20); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation”; Role: Principal Investigator; Awarded 260,000 service units (>25 million CPU hours and 3,000,000 GPU hours) at the Oak Ridge Leadership Computing Facility.
3. 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.**

4. 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**.
5. 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.
6. 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.
7. 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.
8. 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.
9. 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 (2019 – 2021)
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. Innovative and Novel Computational Impact on Theory and Experiment (INCITE) award from the Department of Energy Office of Science (2010)
9. La Jolla Interfaces in Science Postdoctoral Fellowship, Burroughs Wellcome Fund (2005 – 2007)
10. Chemical Computing Group Excellence Award from the American Chemical Society (2003)
11. Chemistry Department Chairman’s Award from the University of Pennsylvania (2000)
12. Chemistry Department Teaching Award from Carnegie Mellon University (1999)

C.3 Recognition and Media Coverage

1. Coverage of a publication in *Nature Communications* (2020),
doi:10.1038/s41467-020-19165-2
Altmetric score 16. 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”.
2. 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 4,371st) of the 118,590 tracked articles of a similar age in all journals and in the **85th percentile** (ranked 2nd) 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”.

3. 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*.

4. Coverage of a publication in *Nature* (2016), doi:10.1038/nature17970

Altmetric score 135. The article is in the **98th percentile** (ranked 3,654th) of the 227,366 tracked articles of a similar age in all journals and in the **60th percentile** (ranked 388th) 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”.

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

Altmetric score 201. The article is in the **99th percentile** (ranked 1,781st) of the 190,421 tracked articles of a similar age in all journals and in the **94th percentile** (ranked 37th) of the 713 tracked articles of a similar age in *Nature Communications*.

6. 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.

7. 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>).

8. 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>).

9. 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. 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)*, 2021
2. Emerging unified description of transcription initiation from cryo-EM and integrative computational modeling. *Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy* 2021
3. 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
4. DNA sculpting as a strategy for base extrusion and damage selection by the repair glycosylase TDG. *Lawrence Berkeley National Laboratory, Berkeley, CA* 2018
5. Lesion search and base extrusion strategy of thymine DNA glycosylase. *Third Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer*, Cancun, Mexico 2018
6. Modeling biological assemblies from low to near atomic resolution. *Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands* 2016
7. 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
8. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct DNA damage response pathways. *Department of Chemistry, Vanderbilt University, Nashville, TN* 2014
9. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct DNA damage response pathways. *Lawrence Berkeley National Laboratory, Berkeley, CA* 2014
10. 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
11. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct functional outcomes in the DNA damage response. *Department of Biochemistry, Emory University, Atlanta, GA* 2013
12. Proliferating cell nuclear antigen and its protein partners in DNA repair. *Department of Biomolecular Sciences, University of Mississippi, Oxford, MS* 2012
13. Integrative modeling of protein/DNA complexes at the replication fork. *Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Minneapolis, MN* 2012
14. Integrative modeling of FEN1 complexes with the sliding clamps PCNA and Rad9-Hus1-Rad1. *Mutagenesis Gordon Research Conference, Newport, RI* 2012
15. 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
16. Integrative modeling of protein/DNA complexes at the replication fork. *Department of Molecular Biology and Biochemistry, Wesleyan University, Middletown, CT* 2011
17. Integrative modeling of protein/DNA complexes at the replication fork. *Conference on Computational Physics (CCP2011)* 2011
18. 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
19. 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*

20. 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*
21. 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*
22. 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*
23. Insight into DNA repair systems from classical and ab initio molecular dynamics. *Department of Chemistry, Columbia University, New York, NY 2007*
24. 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 2007*

C.5 Contributed Presentations (selected out of >70 presentations)

1. Advanced computational modeling of molecular machines involved in transcription initiation. *National Meeting of the American Chemical Society, Atlanta, GA 2021*
2. Transcription initiation machinery functional dynamics and genetic disease. *257th National Meeting of the American Chemical Society, Orlando, FL 2018*
3. Emerging unified description of transcription initiation from cryo-EM and integrative computational modeling. *256th National Meeting of the American Chemical Society, Boston, MA 2018*
4. 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*
5. 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*
6. Integrative modeling of macromolecular assemblies in gene regulation. *Molecular Machines: Integrative Structural and Molecular Biology EMBO Conference, EMBL Heidelberg, Germany 2016*
7. Damage recognition and base extrusion strategies of DNA repair glycosylase enzymes. *251st National Meeting of the American Chemical Society, San Diego, CA 2016*
8. 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*
9. Structurally distinct ubiquitin- and SUMO-modified PCNA: Implications for their distinct roles in the DNA damage response. *Albany 2015 Conference, Albany, NY 2015*
10. Integrative modeling of ubiquitinated and SUMOylated PCNA complexes. *4th Zing Nucleic Acids Conference, Cancun, Mexico 2014*
11. Integrative modeling of protein assemblies involved in transcription. *Biopolymers Gordon Research Conference, Newport, RI 2014*
12. Integrative modeling of complex biological assemblies in DNA replication and transcription coupled repair. *246th National Meeting of the American Chemical Society, Indianapolis, IN 2013*
13. Integrative modeling of ubiquitinated and SUMOylated PCNA complexes. *Nucleic Acids Gordon Research Conference, Biddeford, ME 2013*
14. 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

- 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

C.6 Ad Hoc Reviewer

Science, Proceedings of the National Academy of Science USA, Journal of the American Chemical Society, Nucleic Acids 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 (Northwestern), Stephen J. Benkovic (Pennsylvania State), Walter Chazin (Vanderbilt), 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)

D. TEACHING AND MENTORING

D.1 Courses Taught

- Physical Chemistry II (2010 – 2018; advanced undergraduate/graduate level)
- Quantum Chemistry (2019 – 2021; advanced undergraduate/graduate level; developed an **online version** of this course and taught it in 2020 and 2021)
- Physical chemistry I (2010 – 2019; advanced undergraduate/graduate level)
- Thermodynamics and Chemical Kinetics (2019 – 2020; advanced undergraduate/graduate level)
- Instrumental methods in Spectroscopy (2010 – 2015; advanced undergraduate laboratory)
- Biophysical Chemistry (2012 – 2020; graduate level; team taught with other biophysical division faculty)
- Seminars in Chemistry (2011 – 2016; advanced undergraduate/graduate level; formal course based on the Chemistry Department seminar program)
- Directed Research in Chemistry (2010-2020)
- Undergraduate Research in Chemistry (2010 – 2021)

D.2 Training and Mentoring

Postdoctoral Scholars

- Dr. Chunli Yan (current)
- Dr. Ashutosh Shandilya (current)
- 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

Jina Yu (current)

Thomas Dodd (Ph.D. awarded)

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)

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

E. SERVICE (selected contributions)

2020 – Present	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