CURRICULUM VITAE

Ivaylo Ivanov

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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)
Carnegie Mellon University, Pittsburgh, PA

B.S. in Chemistry (1996)
Sofia University "St. Kliment Ohridski", Sofia, Bulgaria

B. PROFESSIONAL APPOINTMENTS

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

C. SCHOLARSHIP

C.1 Research support

C.1.1 Research Funding

1. National Institutes of Health R01 GM110387 (09/01/15 - 08/31/20); Title: “Integrative Modeling of PCNA Assemblies Engaged in Genome Duplication and Repair”; Role: Principal Investigator; Total cost: $1,675,000
2. Cleon C. Arrington Research Initiation Grant (07/01/18-6/30/19); Title: “Uncovering the Complex Interplay of DNA Repair and Epigenetic Regulation in Genome Maintenance”; Role: Principal Investigator; Total cost: $20,000
3. National Institutes of Health R01 GM126154; (04/01/2018-12/31/2021) Title: “Mechanism and Inhibition of Protein Arginine Methylation”; Role: Co-Investigator; Total cost: $160,000 (to I.I.)
4. National Science Foundation CAREER Award MCB-1149521 (05/01/12 - 04/30/18); Title: “Modeling Assemblies and Interactions at the Replication Fork: Sliding Clamps and Clamp Loaders”; Role: Principal Investigator; Total cost: $824,000
5. National Institutes of Health R01 CA118113-06A1; (06/01/14-5/31/19) Title: “p68 and Ca-Calmodulin Interaction in Cell Migration”; Role: Co-Investigator; Direct cost: $40,000 (to I.I.)
6. Cleon C. Arrington Research Initiation Grant (02/01/11-6/30/12); Title: “Modeling Assemblies and Interactions in Eukaryotic Clamp Loading”; Role: Principal Investigator; Total cost: $10,000

C.1.2 Computational support at the national supercomputing facilities

1. Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award (01/01/2020 - 12/31/21); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation”; Role: Principal Investigator; Awarded 260,000 service units on the OLCF Summit machine (>25 million CPU hours and 3,000,000 GPU hours). 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 (01/01/2019 - 12/31/19); Title: “Advanced Computational Modeling of Molecular Machines in Gene Regulation”; Role: Principal Investigator; Awarded 220,000 service units on the OLCF Summit machine (~198 million CPU hours). The value of an INCITE award for a single project typically exceeds a million dollars.
3. NSF/XSEDE program CHE110042 (4/01/19 - 3/31/20); Title: “Integrative Modeling of Complex Biological Assemblies”; Role: Principal Investigator; Awarded 2,154,00 CPU hours on TACC Stampede 2. The value of the awarded resources is $34,942.
4. NSF/XSEDE program CHE110042 (10/01/17 - 9/30/18); Title: “Integrative Modeling of Complex Biological Assemblies”; Role: Principal Investigator; Awarded 2,240,000 CPU hours and 81,000 GPU node hours. The value of the awarded resources is $58,429.
5. ERCAP DOE Production Award at NERSC (01/07/18 - 01/05/19); Title: “Integrative Modeling of Protein/DNA Complexes at the Replication Fork”; Role: Principal Investigator; Awarded 1,000,000 CPU hours
6. ERCAP DOE Production Award at NERSC (01/07/17 - 01/05/18); Title: “Integrative Modeling of Protein/DNA Complexes at the Replication Fork”; Role: Principal Investigator; Awarded 6,000,000 CPU hours
7. NSF/XSEDE program CHE110042 (04/01/16 - 9/30/17); Title: “Integrative Modeling of Complex Biological Assemblies”; Role: Principal Investigator; Awarded 6,275,000 CPU hours. The value of the awarded resources is $215,334.

8. ERCAP DOE Production Award at NERSC (01/07/16 - 01/05/17); Title: “Integrative Modeling of Protein/DNA Complexes at the Replication Fork”; Role: Principal Investigator; Awarded 3,600,000 CPU hours
9. NSF/XSEDE program CHE110042 (10/01/14 - 9/30/15); Title: “Integrative Modeling of Complex Biological Assemblies”; Role: Principal Investigator; Awarded 6,703,000 CPU hours. The value of the awarded resources is $251,899.
10. ERCAP DOE Production Award at NERSC (01/07/15 - 12/31/15); Title: “Integrative Modeling of Protein/DNA Complexes at the Replication Fork”; Role: Principal Investigator; Awarded 2,200,000 CPU hours
11. 2013 ASCR Leadership Computing Challenge Award (07/01/2013-12/31/2014); Title: “Exploring the Chemical Landscape for Base Excision DNA Repair”; Role: Principal Investigator; Awarded 3,000,000 CPU hours
12. ERCAP DOE Production Award at NERSC (01/07/14 - 01/05/15); Title: “Integrative Modeling of Protein/DNA Complexes at the Replication Fork”; Role: Principal Investigator; Awarded 4,000,000 CPU hours
13. NSF/XSEDE program CHE110042 (10/01/12 - 12/31/13); Title: “Integrative Modeling of Complex Biological Assemblies”; Role: Principal Investigator; Awarded 4,726,000 CPU hours
14. ERCAP DOE Production Award at NERSC (01/07/12 - 01/05/13); Title: “Integrative Modeling of Protein/DNA Complexes at the Replication Fork”; Role: Principal Investigator; Awarded 2,000,000 CPU hours
15. NERSC Initiative for Scientific Exploration (NISE) Award (05/01/11 - 04/30/12); Title: “An Integrative Strategy to Model Complex Biological Assemblies”; Role: Principal Investigator; Awarded 960,000 CPU hours
16. Computational time on the special purpose Anton machine at the National Resource for Biomedical Supercomputing (NRBSC) in Pittsburgh (09/01/11 - 06/30/12); Title: “Modeling connexin hemichannels important for intercellular communication”; Role: Principal Investigator; Awarded 50,000 CPU hours
17. Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award BIP007 (01/01/2009 - 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

C.2 Publications (58 publications, cited >2500 times in Google Scholar, h-index 28)

1. 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) (submitted)
2. 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) (in press)
3. 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
4. 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**)
5. 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

6. 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
7. 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
8. 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
9. 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
10. 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
11. 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**)
12. 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
13. 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
14. 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 >100 times**)
15. 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 αvβ3 at a novel site by rational protein design. *Nature Communications* (2016) **7**, 11675, doi:10.1038/ncomms11675
16. 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
17. 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.jpcb.6b02082 (**Invited article for the J. Andrew McCammon Festschrift special issue**)
18. 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

19. 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

20. 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

21. 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

22. 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

23. 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

24. 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

25. 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

26. 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

27. Tsutakawa, S. E., Shin, D. S., Mol, C. D., Izumi, T., Arvai, A. S., Mantha, A. K., Szczesny, B., **Ivanov, I.** N., 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

28. **Ivanov, I.*** Enzyme cofactors: Double-edged sword for catalysis. *Nature Chemistry* (2013) **5**, 6-7, doi:10.1038/nchem.1529

29. 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**)

30. 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

31. 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)

32. 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 (**Faculty of 1000 recommended Factor 8.0**; **highlighted by the Oak Ridge Leadership Computing Facility** at http://www.olcf.ornl.gov/2011/11/09)

33. 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
34. 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
35. 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**)
36. 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)
37. 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
38. 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**)
39. 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 >100 times**)
40. 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
41. **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
42. **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
43. 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
44. 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
45. 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
46. **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**)

47. **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
48. **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
49. **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
50. 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**)
51. **Ivanov, I.** Terascale ab initio molecular dynamics simulations of proton transfer and dissociation processes in chemical and biological systems. (2004) *ProQuest* AAI3152059
52. 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
53. **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
54. 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
55. 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 >300 times**)
56. **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
57. 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
58. 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
59. **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 papers for which I am a corresponding author

C.3 Selected Awards

1. Innovative and Novel Computational Impact on Theory and Experiment (INCITE) award from the Department of Energy Office of Science (2019-2020)

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.4 Invited Presentations

1. Emerging unified description of transcription initiation from cryo-EM and integrative computational modeling. *Southeast Regional Meeting of the American Chemical Society (SERMACS)*, Augusta, GA **2018**
2. DNA sculpting as a strategy for base extrusion and damage selection by DNA repair glycosylases. *Southeast Regional Meeting of the American Chemical Society (SERMACS)*, Augusta, GA **2018**
3. DNA sculpting as a strategy for base extrusion and damage selection by the repair glycosylase TDG. *Lawrence Berkeley National Laboratory*, Berkeley, CA **2018**
4. Lesion search and base extrusion strategy of thymine DNA glycosylase. *Third Fusion Conference: Dynamic Structures in DNA Damage Responses and Cancer,* Cancun, Mexico **2018**
5. Modeling biological assemblies from low to near atomic resolution. *Van't Hoff Institute for Molecular Sciences, University of Amsterdam,* Amsterdam, The Netherlands **2016**
6. 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**
7. DNA sculpting as a strategy for base extrusion and damage selection by DNA repair glycosylases. *Southeast Regional Meeting of the American Chemical Society (SERMACS)*, Nashville, TN **2014**
8. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct DNA damage response pathways. *Department of Chemistry, Vanderbilt University*, Nashville, TN, GA **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. Integrative modeling of complex biological assemblies in DNA replication and transcription coupled repair. *Southeast Regional Meeting of the American Chemical Society (SERMACS)*, Atlanta, GA **2013**

12. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct functional outcomes in DNA damage response. *Department of Biochemistry, Emory University*, Atlanta, GA **2013**
13. Proliferating cell nuclear antigen and its protein partners in DNA repair. *Department of Biomolecular Sciences, University of Mississippi*, Oxford, MS **2012**
14. Integrative modeling of protein/DNA complexes at the replication fork. *Department of Biochemistry, Molecular Biology and Biophysics*, *University of Minnesota*, Minneapolis, MN **2012**
15. Integrative modeling of FEN1 complexes with the sliding clamps PCNA and Rad9-Hus1-Rad1. *Mutagenesis Gordon Research Conference*, Newport, RI **2012**
16. Solution phase X-ray scattering and multiscale computational modeling reveal the structural dynamics of ubiqutinated PCNA. *Symposium in Honor of J. Andrew McCammon, 243rd National Meeting of the American Chemical Society*, San Diego, CA **2012**
17. Integrative modeling of protein/DNA complexes at the replication fork. *Center for Diagnostics and Therapeutics (CDT), Georgia State University*, Atlanta, GA **2012**
18. Integrative modeling of protein/DNA complexes at the replication fork. *Department of Molecular Biology and Biochemistry, Wesleyan University*, Middletown, CT **2011**
19. Integrative modeling of protein/DNA complexes at the replication fork. *Conference on Computational Physics (CCP2011)* **2011**
20. Integrative modeling of protein/DNA complexes at the replication fork. *Lawrence Berkeley National Laboratory*, Berkeley, CA **2011**
21. 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**
22. 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**
23. 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**
24. 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**
25. The three-metal-ion catalytic mechanism of the DNA repair enzyme endonuclease IV. *Protein Dynamics and Catalysis Conference*, Tarrytown, NY **2008**
26. High performance computing in molecular simulation and computational structural biology. *13th Annual San Diego Supercomputer Center Summer Institute*, La Jolla, CA **2007**
27. 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**
28. Insight into DNA repair systems from classical and ab initio molecular dynamics. *Department of Chemistry, Columbia University*, New York, NY **2007**
29. 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**
30. *Workshop on Petascale Computing in the Biosciences, National Science Foundation*, Arlington, VA **2006** (Invited participant, **contributor to the final report**)

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

31. Transcription initiation machinery functional dynamics and genetic disease. *257th National Meeting of the American Chemical Society,* Orlando, FL **2018**
32. Emerging unified description of transcription initiation from cryo-EM and integrative computational modeling. *256th National Meeting of the American Chemical Society,* Boston, MA **2018**
33. Electron microscopy and integrative modeling shed light on the structures of transcription pre-initiation complexes and the mechanisms of transcription initiation. *National Meeting of the Biophysical Society,* San Francisco, CA **2018**
34. 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**
35. Electron microscopy and integrative modeling shed light on the structures of transcription pre-initiation complexes and the mechanisms of transcription initiation. *Southeast Regional Meeting of the American Chemical Society (SERMACS)*, Charlotte, NC **2017**
36. 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**
37. Integrative modeling of macromolecular assemblies in gene regulation. *Molecular Machines: Integrative Structural and Molecular Biology EMBO Conference,* EMBL Heidelberg, Germany **2016**
38. Integrative modeling of macromolecular assemblies in gene regulation. *5th Zing Nucleic Acids Conference*, Tampa, FL **2016**
39. Damage recognition and base extrusion strategies of DNA repair glycosylase enzymes. *251st National Meeting of the American Chemical Society*, San Diego, CA **2016**
40. 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**
41. Structurally distinct ubiquitin- and SUMO-modified PCNA: Implications for their distinct roles in the DNA damage response. *Albany 2015 Conference*, Albany, NY **2015**
42. Integrative modeling of ubiquitinated and SUMOylated PCNA complexes. *4th Zing Nucleic Acids Conference* Cancun, Mexico **2014**
43. Integrative modeling of protein assemblies involved in transcription. *Biopolymers Gordon Research Conference*, Newport, RI **2014**
44. Integrative modeling of ubiquitinated and SUMOylated PCNA complexes. *Annual Meeting of the Biophysical Society*, San Francisco, CA **2014**
45. Integrative modeling of complex biological assemblies in DNA replication and transcription coupled repair. *246th National Meeting of the American Chemical Society*, Indianapolis, IN **2013**
46. Integrative modeling of ubiquitinated and SUMOylated PCNA complexes. *Nucleic Acids Gordon Research Conference*, Biddeford, ME **2013**
47. 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**
48. 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**

49. Integrative modeling of protein/DNA complexes at the replication fork. *243rd National Meeting of the American Chemical Society*, San Diego, CA **2012**
50. Structure and dynamics of the ternary complexes of FEN1/PCNA/DNA and FEN1/Rad9-Rad1-Hus1/DNA. *Eukaryotic DNA Replication & Genome Maintenance meeting*, Cold Spring Harbor Laboratory, NY **2011**
51. 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**
52. Multiple states of covalently bound ubiquitin on PCNA. *Keystone meeting on DNA Replication and Recombination*, Keystone, CO **2011**
53. Multiple states of covalently bound ubiquitin on PCNA. *Gordon Research Conference DNA Damage, Mutation & Cancer*, Ventura, CA **2010**
54. Specific recognition of the ring-opened state of proliferating cell nuclear antigen by replication factor C promotes eukaryotic clamp-loading. *Biology department seminar*, Georgia State University, Atlanta, GA **2010**
55. Specific recognition of the ring-opened state of proliferating cell nuclear antigen by replication factor C promotes eukaryotic clamp-loading. *24th Annual Symposium of the Protein Society*, San Diego, CA **2010**
56. Specific recognition of the ring-opened state of proliferating cell nuclear antigen by replication factor C promotes eukaryotic clamp-loading. *240th National Meeting of the American Chemical Society*, Boston, MA **2010**
57. Phosphoryl transfer in solution and in enzymatic active sites: Insights from ab initio molecular dynamics. *Algorithms in Macromolecular Modeling (AM3) meeting*, Austin, TX **2009**
58. The interplay of AAA+ molecular machines and sliding clamps at the DNA replication fork. *Institute for Mathematics and its Applications, University of Minnesota*, Minneapolis, MN **2009**

C.6 Ad hoc reviewer for the following journals

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 Collaborators in the past 5 years

Eva Nogales (UC-Berkeley)

Yuan He (Northwestern University)

Stephen J. Benkovic (Pennsylvania State University)

Walter Chazin (Vanderbilt University)

Y. George Zheng (University of Georgia)

Eric Ortlund (Emory University)

Samir Hamdan (KAUST)

Susan Tsutakawa (Lawrence Berkeley National Laboratory)

John A. Tainer (University of Texas M.D. Anderson Cancer Center)

Zhihao Zhuang (University of Delaware)

M. Todd Washington (University of Iowa)

Zhi-ren Liu (Georgia State University)

Dong Wang (University of California, San Diego)

Yves Pommier (NIH)

David Wilson (Georgia State University)

C.8 Society Memberships

American Chemical Society (since 1999)

Biophysical Society (since 2004)

Protein Society (since 2004)

Sigma Xi (Full membership since 2004)

C.9 Media Coverage

1. 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”.

2. 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.*

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

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

4. 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*.

5. 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 96 percentile of the 252241 tracked articles of a similar age in all journals and in the 76 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.

6. 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/researchers-show-how-proteins-help-dna-replicate-past-a-damaged-site).

7. 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).

8. 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/supercomputers-simulate-the-molecular-machines-that-replicate-and-repair-dna/).

D. TEACHING, INCLUDING ADVISING

D.1 Courses Taught (as Instructor of Record)

1. Physical Chemistry II (Level: Advanced Undergraduate/Graduate): spring semester 2010, spring

semester 2011, spring semester 2013, spring semester 2014, spring semester 2016, fall semester 2016, spring semester 2017, fall semester 2017, fall semester 2018, fall semester 2019

2. Physical chemistry I (Level: Advanced Undergraduate/Graduate): fall semester 2010, spring semester 2012, spring semester 2015, spring semester 2019
3. Instrumental methods III (Level: Advanced Undergraduate/Graduate), Spectroscopy lab: fall semester 2010, fall semester 2011, fall semester 2012, fall semester 2013, fall semester 2014, fall semester 2015
4. Biophysical Chemistry (Level: Graduate): fall semester 2012, fall semester 2014, fall semester 2016, fall semester 2018
5. Dissertation Research in Chemistry: spring semester 2011, summer semester 2011, fall semester 2011, spring semester 2012, summer semester 2012, fall semester 2012, spring semester 2013, summer semester 2013, fall semester 2013, spring semester 2014, summer semester 2014, fall semester 2014, spring semester 2015, summer semester 2015, fall semester 2015, spring semester 2016, summer semester 2016, fall semester 2016, spring semester 2017, summer semester 2017, fall semester 2017, spring semester 2018, summer semester 2018, fall semester 2018, spring semester 2019
6. Chemistry Laboratory I (Undergraduate Research): summer semester 2011, fall semester 2011, summer semester 2012, fall semester 2013, summer semester 2014, fall semester 2014, summer semester 2015, fall semester 2015, spring semester 2016, summer semester 2016, fall semester 2016, spring semester 2017, summer semester 2018, spring semester 2019
7. Chemistry Laboratory II (Undergraduate Research): fall semester 2011, spring semester 2012, fall semester 2012, fall semester 2014
8. Seminars in Chemistry (Level: Advanced Undergraduate/Graduate): fall semester 2011, spring semester 2012, fall semester 2012, spring semester 2013, fall semester 2013, spring semester 2014, fall semester 2014, spring semester 2015, fall semester 2015, spring semester 2016
9. Directed Research in Chemistry: summer semester 2010, fall semester 2010, spring semester 2011, spring semester 2012, summer semester 2012, fall semester 2012, spring semester 2013, summer semester 2013, fall semester 2013, spring semester 2014, summer semester 2014, fall semester 2014, spring semester 2015, summer semester 2015, fall semester 2015, summer semester 2016, fall semester 2016, spring semester 2017

D.2 Training and Mentoring

Postdoctoral Scholars

Dr. Chunli Yan (current)

Dr. Ashutosh Shandilya (current)

Dr. Kathleen Carter (subsequently postdoc at Emory University)

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

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

Graduate students

Thomas Dodd (current)

Kurt Martin (current)

Jina Yu (current)

Zhenyu Wang, completed a M.S. thesis entitled “Computational Study of Protein Arginine

Methyl-Transferases (PRMTs)"

Dr. Kathleen Carter, completed a Ph.D. dissertation "Insights into the Association of Proteins and Small Molecules with the Minor Groove of DNA"

Bernard Scott, completed a M.S. thesis entitled "Computational Studies of Liver Receptor Homolog 1 in the Presence of Small Molecule Agonists: Allosteric Communication and Virtual Screening for New Potential Drug Candidates" (subsequently at the University of Utah)

Dr. Bradley R. Kossmann, completed a Ph.D. dissertation "Computational Investigations of Biomolecular Motions and Interactions in Genomic Maintenance and Regulation" (subsequently employed as a Senior Data Scientist at 360i company in Atlanta, GA)

Dr. Xiaojun Xu, completed a Ph.D. dissertation "Modeling Assemblies and Interactions at the Replication Fork: Sliding Clamps and Clamp Interacting Enzymes" (subsequently ORISE Fellow at the CDC and fellow at the La Jolla Institute of Allergy and Immunology)

Shih-Wei Chuo, completed a M.S. thesis entitled "Discovery of Potent Tyrosyl-DNA Phosphodiesterase 1 Inhibitors Using in silico Virtual Screening & Network Analysis for Evolution of Allosteric Communication in 3-ketosteroid Receptors" (subsequently at the University of California, Davis)

Stephanie Kofsky, graduated with a M.S. degree and accepted position at Kemira, Atlanta, GA

Patrick Chepaitis, graduated with a M.S. degree

Yang Zhen, graduated with a M.S. degree

Undergraduate student researchers

Fernando Cortez (spring/summer of 2010; **hosted as McNair Scholar**)

Amanuel Gebremariam (summer 2011; fall 2011; spring 2012)

Oladayo Agboola (fall 2011; spring 2012)

Bao-Khanh Ho (fall 2011)

Syiedah Korre (fall 2011)

Yosef Mekuria (summer and fall 2012)

Evan Sinyard (fall 2013)

Albertha Sabree (summer 2014; **NSF REU program trainee**)

Eric Zientowski (summer, fall 2014)

Zachary Ferris (fall, 2014)

Annie Yoon (fall, 2015)

Zacharia Robow (summer, fall 2015)

Thomas Dodd (fall 2015, spring 2016)

Lily Vassileva (fall 2016, spring 2017, summer 2017)

Nicole Ogbomoh (summer 2016, fall 2016)

Sam Delmerico (spring 2017, summer 2017)

Maia Wells (summer 2017, fall 2018)

Student Awards

Molecular Basis of Disease Doctoral Fellowship to Xiaojun Xu

Dean's Doctoral Fellowship to Kathleen Carter

National XSEDE (Extreme Science and Engineering Discovery Environment) Scholarship to Bernard Scott

Molecular Basis of Disease Doctoral Fellowship to Kurt Martin

Molecular Basis of Disease Doctoral Fellowship to Tom Dodd

Molecular Basis of Disease Doctoral Fellowship to Bradley R. Kossmann

Molecular Basis of Disease Travel Fellowship to Bradley R. Kossmann

Award for Outstanding Research at the Ph.D. level to Bradley R. Kossmann

Molecular Basis of Disease Outstanding Fellow Award to Bradley R. Kossmann

Hopkins Endowed Fellowship in Biophysical Chemistry to Tom Dodd

Molecular Basis of Disease Outstanding Fellow Award to Tom Dodd

E. SERVICE

2018	Panelist at the 2018 Scientific Computing Day at GSU
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 NIH/CSR
2016-Present	Reviewing Editor, Frontiers Journals in Physics, Physiology and Molecular Biosciences
2015-2017	Member of the University Senate, Georgia State University, Atlanta, GA
2015-2017	Member, Senate Admissions & Standards Committee, Georgia State University, Atlanta, GA
2015-2017	Member, Senate Planning & Development Committee, Georgia State University, Atlanta, GA
2014-Present	Member, Computer Support Committee, Department of Chemistry, Georgia State University, Atlanta, GA
2014	Reviewer on the Genetics, Genomics, Proteomics panel of the NSF Graduate Research Fellowship Program (GRFP)
2013-Present	Reviewer for regular NSF and NSF-CAREER proposals submitted to the MCB division of the National Science Foundation (Genetic Mechanisms Cluster)
2013	Assisted with the organization of the "Third International Conference on Chemical and Structural Biology of Nucleic Acids and Proteins for Novel Drug Discovery" (Sep. 13-15, 2013, Atlanta, USA).

2013	Panelist at an NSF-CAREER award workshop organized by University Research Services and Administration (URSA)
2011-2016	Coordinator for the Chemistry Department seminar series
2010-Present	Library Liaison, Department of Chemistry, Georgia State University, Atlanta, GA
2009-Present	Member, Petitions/Awards Committee, Department of Chemistry, Georgia State University, Atlanta, GA
2009-Present	Member, Biophysical Chemistry Doctoral Preliminary Exam Committee, Department of Chemistry, Georgia State University, Atlanta, GA