

Curriculum Vitae

Ivaylo Ivanov

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A. Education:

University of Pennsylvania, Philadelphia, PA	<i>Ph.D. in Chemistry</i>	12/2004
Carnegie Mellon University, Pittsburgh, PA	<i>M.S. in Chemistry</i>	05/1999
Sofia University "St. Kliment Ohridski", Sofia, Bulgaria	<i>B.S. in Chemistry</i>	06/1996

B. Appointments:

2009 – Present	Assistant Professor, Dept. of Chemistry (joint appointment Dept. of Biology) Georgia State Univ., Atlanta, GA
2009 – Present	Faculty Member, Molecular Basis of Disease Program at Georgia State Univ.
2009 – Present	Faculty Member, Center for Biotechnology and Drug Design
2005 – 2009	Postdoctoral Scholar, Department of Chemistry & Biochemistry, University of California, San Diego and the Scripps Research Institute (mentors: Prof. J. Andrew McCammon and Prof. John Tainer)
1999 – 2004	Research Associate, Department of Chemistry, Univ. of Pennsylvania (advisor: Prof. Michael L. Klein)

C. Publications (27 published papers, cited 566 times in ISI Science Citation Index database, h-index 15).

1. Tsutakawa, S.E.; Van Wynsberghe, A.; 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 (in press *Proceedings of the National Academy of Sciences U.S.A.*)
2. Guardiani C.; Feng Y.; Xu X.; Zheng Y.G.; Ivanov I.^{*†} Interplay between acetylation and methylation in histone H4 tail: A structural perspective (submitted)
3. Wang J. et al.[†] Histone H4 acetylation differentially modulates arginine methylation by an in Cis mechanism *Journal of Biological Chemistry* doi:10.1074/jbc.M110.207258
4. Cheng X.; Ivanov, I.[†] Molecular dynamics and computational toxicity (review article submitted to *Methods in Molecular Biology - Computational Toxicity*)
5. Fritsch, S.; Ivanov, I.; Wang H.L.; Cheng X.[†] Ion selectivity mechanism in a bacterial pentameric ligand gated ion channel *Biophysical Journal* **2011**, *100*, 390-398
6. Balle et al.[†] New insights into the GABAA receptor structure and orthosteric ligand binding: Receptor modeling guided by experimental data *Proteins: Structure, Function and Bioinformatics* doi: 10.1002/prot.22975
7. Tainer, J. A.; McCammon, J. A.; Ivanov, I.^{*†} Specific recognition of the ring-opened state of proliferating cell nuclear antigen by replication factor C promotes eukaryotic clamp-loading *J. Am. Chem. Soc.* **2010**, *132*, 7372. (highlighted by the National Center for Computational Sciences(NCCS) at <http://www.nccs.gov/2010/06/24>)
8. Cheng, X.; Ivanov, I.; Hailong, W.; 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.
9. 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*, 4702-9.

*corresponding author; † since joining GSU

10. Som A.; Vemparala S.; Ivanov I.; Tew G. N. Synthetic mimics of antimicrobial peptides. *Peptide Science (Biopolymers)* **2008**, *90*, 83-93.
11. Gorfe, A.; Chang, C.; Ivanov, I.; McCammon, J.A. Dynamics of the acetylcholine esterase tetramer *Biophysical Journal* **2008** *94*, 1144-1154.
12. Ivanov, I.*; Cheng, X.; Sine, S. M.; McCammon, J. A. Barriers to ion translocation in cationic and anionic receptors from the Cys-loop family *J. Am. Chem. Soc.* **2007** *129*, 8217-8224.
13. Cheng, X.; Ivanov, I.*; Hailong, W.; Sine, S. M.; McCammon, J. A. Nanosecond time scale conformational dynamics of the human $\alpha 7$ nicotinic acetylcholine receptor *Biophys. J.* **2007** *93*, 2622–2634.
14. 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 U.S.A.* **2007** *104*,1465-70.
15. Ivanov, I.*; Chapados B.; McCammon, J. A.; Tainer, J. A. Proliferating cell nuclear antigen loaded onto double-stranded DNA: Dynamics and minor groove interactions *Nucleic Acids Research* **2006** *34*, 6023-33.
16. 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 *Journal of the American Chemical Society* **2006** *128*, 1778-1779.
17. Vemparala, S.; Ivanov, I.; Pophristic, V.; Spiegel, K.; DeGrado, W. F.; Klein, M. L. Ab initio calculations of intra bond parameters for a class of arylamide polymers *Journal of Computational Chemistry* **2006** *27*, 693.
18. 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*, 3517-3526.
19. Ivanov, I.*; Raugei, S.; Chen, B.; Klein, M. L. Relative pK_a values from first-principles molecular dynamics: the case of histidine deprotonation *Journal of Physical Chemistry B* **2006** *110*, 6365-6371.
20. Choi, S.; Clements, D. J.; Pophristic, V.; Ivanov, I.; Vemparala, S.; Bennett, J. S.; Klein, M. L.; Winkler, J. D.; and DeGrado, W. F. The design and evaluation of heparin-binding foldamers *Angew. Chemie* **2005** *44*, 6685. (featured on the **cover of Angewandte Chemie**)
21. Ivanov, I.*; Klein, M. L. Dynamical flexibility and proton transfer in the arginase active site probed by ab initio molecular dynamics methods *J. Am. Chem. Soc.* **2005** *127*, 4010.
22. 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 *Biophys. J.* **2004** *87*, 2107.
23. Ivanov, I.*; Klein, M. L. First principles computational study of the active site of arginase *Proteins* **2004** *54*,1.
24. Chen, B.; Ivanov, I.; Klein, M. L.;Parrinello, M. Hydrogen bonding in water *Phys. Rev. Lett.* **2003** *91*, 215503. (**cited over 100 times** according to the ISI database)
25. Min, G. et al. Solution characterization of monodisperse atactic polystyrenes by static and dynamic light scattering *Int. J. Pol. Anal. Char.* **2003** *8*, 187.
26. Ivanov, I.*; Klein, M. L. Deprotonation of a histidine residue in aqueous solution using constrained ab initio molecular dynamics *J. Am. Chem. Soc.* **2002** *124*, 13380.
27. 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 solution *J. Phys. Chem. B* **2002** *106*, 12006.
28. Chen, B.; Park, J. M.; Ivanov, I.; Parrinello, M.; Klein, M. L. First-principles study of aqueous hydroxide solutions *J. Am. Chem. Soc.* **2002** *124*, 8534.
29. Ivanov, I.; Gherman, B. F.; Yaron, D. Comparison of the INDO band structures of polyacetylene, polythiophene, polyfuran, and polypyrrole *Synthetic Metals* **2001** *116*, 111.

D. Synergistic Activities

Teaching - Physical Chemistry I and II, Computational Chemistry (guest lecturer), Spectroscopy Laboratory

Mentoring (group members): three postdoctoral fellows (current: Dr. Buddhadev Maiti and Dr. Chunli Yan; recent: Dr. Carlo Guardiani), two graduate students (Xiaojun Xu and Yang Zhen) and several undergraduate students

Selected Awards:

- 2011 DOE NERSC Initiative for Scientific Exploration (NISE) Award 'An Integrative Strategy to Model Complex Biological Assemblies' (960,000 CPU hours)
- 2011 Cleon C. Arrington Research Initiation Grant, Georgia State Univ.
- 2011 NSF/Teragrid CHE110042 'Exploring the Chemical Landscape for Base Excision DNA Repair' (2,500,000 CPU hours)
- 2008-2010 INCITE award from the DOE Office of Science entitled '*Interplay of AAA+ Molecular Machines, DNA Repair Enzymes and Sliding Clamps at the Replication Fork: A Multiscale Approach to Modeling Replisome Assembly and Function*' (6.5 million CPU hours)
- 2006-2007 Principal Investigator on a renewed LRAC award (over 1 million CPU hours)
- 2006 UCSD Nominee for a Burroughs Wellcome Fund Career Award at the Scientific Interface (selected among candidates from all university divisions)
- 2005 Principal Investigator on a NSF LRAC (Large Resource Allocation Committee) award entitled '*Large Scale Classical and Ab Initio Molecular Dynamics Simulations of Enzymes and Supramolecular Assemblies Involved in DNA Repair*' (500,000 CPU hours)
- 2005-2007 Burroughs Wellcome Fund (La Jolla Interfaces in Science) Postdoctoral Fellowship
- 2003 Chemical Computing Group Excellence Award, American Chemical Society
- 2000 Chemistry Department Chairman's Award, University of Pennsylvania
- 1999 Chemistry Department Teaching Award, Carnegie Mellon University

Professional Activities:

- Refereed manuscripts for *Science*, *Journal of the American Chemical Society*, *Journal of Physical Chemistry*, *ChemPhysChem*, *Journal of Chemical Theory and Computation*, *Biophysical Journal*, *Chemical Communications*, *Journal of Chemical Physics*, *PLoS Computational Biology*, *PLoS One* and *Journal of Structural Biology* among others.
- **21 invited presentations** (at Oak Ridge National Lab, Georgia Tech, Columbia Univ., UCLA, UCSD, Univ. of Colorado, Johns Hopkins Univ., Princeton Univ. etc.) and over **40 contributed presentations** at professional meetings
- Ivanov, I. High Performance Computing in Molecular Simulation and Computational Structural Biology. 13th Annual San Diego Supercomputer Center Summer Institute 2007, La Jolla, CA (invited guest lecturer)
- Workshop on Petascale Computing in the Biosciences, National Science Foundation, Arlington, VA 2006 (Invited participant, **contributor to the final report**)
- Ivanov I. Visualization of biomolecular dynamics. Iona College, New Rochelle, NY (Invited talk in the Faculty Development Seminar series at a PUI college)
- Ivanov, I. Extending the time and spatial scales in molecular simulation. Iona College, New Rochelle, NY

Society Memberships: American Chemical Society, AAAS, Biophysical Society, Protein Society, Sigma Xi (Full membership)

E. Collaborators

Dr. Susan Tsutakawa (Lawrence Berkeley National Laboratory); Dr. Xiaolin Cheng (Technical Staff Member, ORNL), Prof. Stephen Benkovic (Penn State Univ.), Prof. Manju Hingorani (Wesleyan Univ.); Prof. Steven Sine (Mayo Clinic); Prof. William F. DeGrado (Univ. of Pennsylvania)