

## Curriculum Vitae

### Ivaylo Nikolaev Ivanov

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#### Positions:

Georgia State University, Atlanta, GA	<i>Assistant Professor</i>	2009 – Present
University of California, San Diego and The Scripps Research Institute, La Jolla, CA	<i>Postdoctoral training</i>	2005 – 2009

*Mentors: Dr. J. Andrew McCammon and Dr. John A. Tainer*

#### Education:

University of Pennsylvania, Philadelphia, PA	<i>Ph.D. in Chemistry</i>	12/2004
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*Graduate advisor: Dr. Michael L. Klein*

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

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

#### Research Experience:

**2005 - 2009 University of California-San Diego and The Scripps Research Institute:** Investigated topics related to the maintenance of genomic integrity by ab initio molecular dynamics, classical and combined quantum mechanics/molecular mechanics computations. Explored the global conformational dynamics and energetics of ion permeation in the human  $\alpha 7$  nicotinic acetylcholine receptor.

**1999 - 2004 University of Pennsylvania:** Performed first principles simulations of the enzyme arginase in the context of the broader theme of catalysis by multinuclear metalloenzymes. Studied the utility of the Car-Parrinello method in determining free energies and relative pKa values. Implemented a variant of the fast multipole method in the form of a C++ class library.

**1999 - 2000 IBM T. J. Watson Research Center:** Carried out collaborative research on a new mixed force/domain decomposition approach for the parallelization of the molecular dynamics code PINY.

**1997 - 1999 Carnegie Mellon University:** Carried out research on the electronic structure of conjugated polymers. Performed laser light scattering experiments on polystyrene solutions.

## Awards:

- 2008 Principal Investigator on an 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*' (2 year award; 2.6 million CPU hours in 2009)
- 2007 Principal Investigator on a renewed LRAC award (600,000 CPU hours)
- 2006 Principal Investigator on a renewed LRAC award (half a million CPU hours)
- 2006 UCSD Nominee for a Burroughs Wellcome Fund Career Award at the Scientific Interface (selected among candidates from all university divisions, including the school of engineering, medicine, physical sciences and pharmacology)
- 2005 Principal Investigator on a National Science Foundation 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*' (awarded over half a million 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
- 1992-1996 Scholarship for academic achievement, Sofia University
- Winner of 1991 national chemistry competition (Chemistry Olympiad), Bulgaria

## Society Memberships:

American Chemical Society, American Association for the Advancement of Science, Biophysical Society, Protein Society, Sigma Xi (Full membership)

## Professional Activities:

- Refereed manuscripts for the *Journal of the American Chemical Society*, *Journal of Physical Chemistry*, *ChemPhysChem*, *Journal of Chemical Theory and Computation*, and *Chemical Communications*.

## Past and Present Professional Affiliations:

- Center for Biotechnology and Drug Design (Georgia State University)
- NSF Center for Theoretical Biological Physics (UCSD, Scripps, Salk Institute)
- National Biomedical Computation Resource (UCSD)
- Institute for Complex Adaptive Matter (ICAM)
- Center for Molecular Modeling (UPenn)

## Research Interests:

- Classical and ab initio molecular dynamics of chemical and biological systems.
- Enzyme catalysis mechanisms. DNA replication and repair enzymes. Organization of the replication and repair processes in the cell. Multi-enzyme complexes and supramolecular assemblies involved in DNA replication and repair.
- New algorithms. Hierarchical and multi-scale techniques in molecular dynamics simulation. Mixed quantum-classical systems. Algorithms for efficient sampling on complex free energy landscapes.
- Parallel computation. Development of scaleable parallel algorithms for molecular dynamics.
- Application of coarse-grain methods to study self-assembly processes in chemistry and biology.

**Refereed Publications** (Cited **356** times in ISI Science Citation Index database; h-index **11**):

1. Ivanov, I.; Tainer, J. A.; McCammon, J. A. Specific recognition of the ring-opened state of proliferating cell nuclear antigen by replication factor C promotes eukaryotic clamp-loading (submitted)
2. 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.
3. 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.
4. Som A.; Vemparala S.; Ivanov I.; Tew G. N. Synthetic mimics of antimicrobial peptides. *Peptide Science (Biopolymers)* **2008**, *90*, 83-93. (invited review)
5. Gorfe, A.; Chang, C.; Ivanov, I.; McCammon, J.A. Dynamics of the acetylcholine esterase tetramer *Biophysical Journal* **2008** *94*, 1144-1154.
6. 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.
7. 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 *Biophysical Journal* **2007** *93*, 2622–2634.
8. 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.
9. 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.
10. 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.
11. 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.
12. 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.
13. Ivanov, I.; Raugei, S.; Chen, B.; Klein, M. L. Relative pK<sub>a</sub> values from first-principles molecular dynamics: the case of histidine deprotonation *Journal of Physical Chemistry B* **2006** *110*, 6365-6371. (featured among **the most cited articles in 2006** for the Journal of Physical Chemistry)

14. 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 *Angewandte Chemie-International Edition* **2005** *44*, 6685-6689. (featured on the **cover of Angewandte Chemie**)
15. Ivanov, I.; Klein, M. L. Dynamical flexibility and proton transfer in the arginase active site probed by ab initio molecular dynamics methods *Journal of the American Chemical Society* **2005** *127*, 4010.
16. 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.
17. Ivanov, I.; Klein, M. L. First principles computational study of the active site of arginase *Proteins: Structure, Function, and Bioinformatics* **2004** *54*, 1-7.
18. Chen, B.; Ivanov, I.; Klein, M. L.; Parrinello, M. Hydrogen bonding in water *Physical Review Letters* **2003** *91*, 215503.
19. Min, G. et al. Solution characterization of monodisperse atactic polystyrenes by static and dynamic light scattering *International Journal of Polymer Analysis and Characterization* **2003** *8*, 187-207.
20. 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.
21. Chen, B.; Ivanov, I.; Park, J. M.; Parrinello, M.; Klein, M. L. Solvation structure and mobility mechanism of OH<sup>-</sup>: A Car-Parrinello molecular dynamics investigation of alkaline solution *Journal of Physical Chemistry B* **2002** *106*, 12006-12016.
22. Chen, B.; Park, J. M.; Ivanov, I.; Parrinello, M.; Klein, M. L. First-principles study of aqueous hydroxide solutions *Journal of the American Chemical Society* **2002** *124*, 8534-8535.
23. 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.

#### **Manuscripts in Preparation:**

1. van Wynsberghe, A.\*; Ivanov\*, I.; Tainer, J.A.; McCammon J.A. Multi-scale modeling of PCNA - monoubiquitin interactions (in preparation, \*equal contribution)
2. Ivanov, I.; Noel, J.; Onuchic J.; Tainer, J. A.; McCammon, J. A. Mechanism of sliding clamp opening by the clamp loader RFC: Insight from atomistic and coarse-grain simulation (to be submitted)
3. Ivanov, I.; Cheng, X.; Khavrutskii I.; Tainer J. A.; McCammon, J. A. Base flipping in normal and damaged DNA: a harmonic Fourier bead path optimization approach. (to be submitted)

### **Invited Presentations:**

1. Ivanov I. 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**
2. Ivanov I. The Interplay of AAA+ Molecular Machines and Sliding Clamps at the DNA Replication Fork. Georgia State University, Atlanta, GA **2009**
3. Ivanov I. The Interplay of AAA+ Molecular Machines and Sliding Clamps at the DNA Replication Fork. University of California Los Angeles, Los Angeles, CA **2009**
4. Ivanov I.; Tainer J. A.; McCammon J. A. The Interplay of AAA+ Molecular Machines and Sliding Clamps at the DNA Replication Fork. *Pharmacology Research Discussions*, University of California San Diego, La Jolla, CA **2008**
5. Ivanov, I. and McCammon, J. A. The three-metal-ion catalytic mechanism of the DNA repair enzyme endonuclease IV. *Third CMM Workshop on QM/MM Simulations*, Philadelphia, PA **2008**
6. Ivanov, I. and McCammon, J. A. The three-metal-ion catalytic mechanism of the DNA repair enzyme endonuclease IV. *Protein Dynamics and Catalysis Conference*, Tarrytown, NY **2008**
7. Ivanov, I.; Cheng X.; Sine S. M.; McCammon, J. A. Barriers to ion translocation in cationic and anionic receptors from the cys-loop family. *234<sup>th</sup> National Meeting of the American Chemical Society*, Boston, MA **2007**
8. Ivanov, I. High Performance Computing in Molecular Simulation and Computational Structural Biology. *13<sup>th</sup> Annual San Diego Supercomputer Center Summer Institute 2007*, La Jolla, CA 92093
9. Ivanov, I.; Cheng, X.; McCammon, J. A. Global collective motions and barriers to ion translocation in receptors from the Cys-loop family. *UCSD, Center for Theoretical Biological Physics*, La Jolla CA **2007**
10. Ivanov, I. Insight into DNA repair systems from classical and ab initio molecular dynamics. Johns Hopkins University School of Medicine, Baltimore, MD **2007**
11. Ivanov, I. Insight into DNA repair systems from classical and ab initio molecular dynamics. Columbia University, New York, NY **2007**
12. Ivanov, I. DNA repair systems and ligand-gated ion channels: Insights from classical and ab initio molecular dynamics. Washington University School of Medicine, St. Louis, Missouri **2007**
13. Ivanov I. Visualization of biomolecular dynamics. *Iona College*, New Rochelle, NY **2005** (Faculty Development Seminar series)
14. Ivanov, I.; Klein, M. L. Applications of Car Parrinello molecular dynamics to study chemical processes in solution and at enzymatic active sites. *The Scripps Research Institute*, San Diego, CA **2003**
15. Ivanov, I.; Klein, M. L. Extending the time and spatial scales in molecular simulation. *Princeton University*, Princeton, NJ **2003**
16. Ivanov, I.; Klein, M. L. Extending the time and spatial scales in molecular simulation. *Iona College*, New Rochelle, NY **2003**

**Contributed presentations (selected from ~ 30 presentations):**

17. Ivanov, I.; van Wynsberghe, A.; Tainer, J.A.; McCammon J.A. Multi-scale modeling of PCNA - monoubiquitin interactions *Gordon Research Conference on Nucleic Acids*, Biddeford, ME **2009**
18. Ivanov I. The Interplay of AAA+ Molecular Machines and Sliding Clamps at the DNA Replication Fork. *IMA workshop on molecular dynamics*, Minneapolis, MN **2009**
19. Ivanov, I.; Tainer, J. A.; McCammon, J. A. Mechanism of sliding clamp opening by the eukaryotic clamp loader replication factor C. *236<sup>th</sup> National Meeting of the American Chemical Society*, Philadelphia, PA **2008**
20. Ivanov, I.; Tainer, J. A.; McCammon, J. A. Mechanism of sliding clamp opening by the eukaryotic clamp loader replication factor C. *Annual Meeting of the Protein Society*, San Diego, CA **2008**
21. Ivanov, I.; Cheng, X.; McCammon, J. A. Barriers to ion translocation in the human alpha 7 nicotinic acetylcholine receptor. *51<sup>th</sup> Annual Meeting of the Biophysical Society*, Baltimore, MD **2007**
22. Ivanov, I.; Tainer, J. A.; McCammon, J. A. Ab initio molecular dynamics reveals striking reorganization of the trinuclear metal cluster of endonuclease IV during catalysis. *232<sup>nd</sup> National Meeting of the American Chemical Society*, San Francisco, CA **2006**
23. Ivanov, I.; Tainer, J. A.; McCammon, J. A. Interactions and dynamics of sliding clamp proteins on DNA. *Annual Meeting of the Protein Society*, San Diego, CA **2006**
24. Ivanov, I.; Tainer, J. A.; McCammon, J. A. The three-metal-ion catalytic mechanism of the DNA repair enzyme endonuclease IV. *ICAM workshop on Multi-scale Interactions and Dynamics in Biological Systems*, Washington University School of Medicine, St. Louis, Missouri **2006 (ICAM Junior Travel Award)**
25. Ivanov, I.; Tainer, J. A.; McCammon, J. A. Dynamics of proliferating cell nuclear antigen loaded onto double-stranded DNA. *50<sup>th</sup> Annual Meeting of the Biophysical Society*, Salt Lake City, UT **2006**
26. Ivanov I.; Tainer J. A.; McCammon J. A. Ab initio DFT molecular dynamics: Applications to metalloenzymes. *DFT Discussions*, University of California San Diego, La Jolla, CA **2005** (Mini-symposium in honor of Walter Kohn)
27. Ivanov, I.; Vemparala, S.; Pophristic, V.; Kuroda, K.; Klein, M. L.; De Grado, W. F. Characterization of non-biological antimicrobial polymers in aqueous solution and at water-lipid interfaces from all atom and coarse grained molecular dynamics. *229<sup>th</sup> National Meeting of the American Chemical Society*, San Diego, CA **2005** (Computational Division)
28. Ivanov, I.; Klein, M. L. Proton transfer in the active site of arginase: Insight from ab initio molecular dynamics. *228<sup>th</sup> National Meeting of the American Chemical Society*, Philadelphia, PA **2004**
29. Ivanov, I.; Rauegi S.; Klein, M. L. Effect of ions on the dipole moment and electronic properties of water. *Gordon Research Conference on Computational Chemistry*, Plymouth, NH **2003**
30. Ivanov, I.; Klein, M. L. Structural determinants of the catalytic activity of arginase: Insights from terascale quantum simulations of the arginase active site. *226<sup>th</sup> National Meeting of the American Chemical Society*, New York, NY **2003**
31. Ivanov, I.; Klein, M. L. Weak acid deprotonation in aqueous solution. *Gordon Research Conference*

*on the Chemistry and Physics of Liquids*, Plymouth, NH **2003**

32. Ivanov, I.; Klein, M. L. Relative  $pK_a$  values from first principles molecular dynamics: the case of histidine deprotonation. *225<sup>th</sup> National Meeting of the American Chemical Society*, New Orleans, LA **2003** (Computational Chemistry Division) (**Travel award**)

**Other Conference Participation:**

1. 6<sup>th</sup> Howard Hughes Medical Institute Science Meeting, Janelia Farm Campus, Ashburn, VA **2007**
2. Workshop on Petascale Computing in the Biosciences, National Science Foundation, Arlington, VA **2006 (Invited participant, contributor to the final report)**
3. Regulation of Protein Phosphorylation: Energy Landscapes, Allostery and Dynamic Regulation, Institute for Complex Adaptive Matter (ICAM) Conference, San Diego, CA **2008**
4. Frontiers in signal transduction and protein phosphorylation, Institute for Complex Adaptive Matter (ICAM) Conference, San Diego, CA **2005**
5. Conference on stochastic and multi-scale problems in the sciences, Institute for Advanced Study, Princeton, New Jersey **2002**
6. ES2001 - Thirteenth annual workshop on recent developments in electronic structure algorithms, Princeton University **2001**

## References

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