Dmytro Kosenkov

Purdue University
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Education

Postdoctoral Research, August 2009–Present
Department of Chemistry, Purdue University,
West Lafayette, IN
Mentor: Prof. Lyudmila V. Slipchenko

Ph.D., Chemistry, Jackson State University, August 2009
Jackson, MS
Dissertation: "Thermodynamic and Kinetic Simulations on Biological Molecules in Gas Phase and in Solution: Evaporation, Isomerisation and Hydrogen Bonding"
Advisor: Prof. Jerzy Leszczynski

M. S., Physics, National Taras Shevchenko University of Kyiv, June 2005
Kyiv, Ukraine
Thesis: "Computational Study of Molecular Structure and Hydrogen Bonding in Hypermodified Nucleosides and Nucleotides of Guanine"
Advisor: Dr. Galina I. Dovbeshko

B. S., Physics, National Taras Shevchenko University of Kyiv June 2003
Kyiv, Ukraine

Research Experience

Postdoctoral Research Associate, August 2009–Present
Department of Chemistry, Purdue University,
West Lafayette, IN
Mentor: Prof. Lyudmila V. Slipchenko

Research focus:

- Development of *ab initio* based Effective Fragment Potential (EFP) force-field and its implementation into the Q-Chem electronic structure package.
- Application of the EFP method for QM/MM simulations of UV/Vis spectra of organic chromophores in solvents of different polarity.
- Investigation of effects of intermolecular interactions on electronic excitations in biological chromophores.

Graduate Research Assistant, October 2005–August 2009
Department of Chemistry, Jackson State University,
Jackson, MS

Intern, Spring 2004
Laboratory of X-ray Analysis, Institute for Single Crystals,
National Academy of Science of Ukraine,
Kharkov, Ukraine

Engineer, September 2002–June 2005
Department of Physics of Biological Systems,
Institute of Physics of National Academy of Sciences of Ukraine,
Kyiv, Ukraine

Teaching Experience

Team-Teaching Lecturer Spring 2011
Department of Chemistry, Purdue University,
West Lafayette, IN

Computational Chemistry

Team-Teaching Lecturer Fall 2010-2011
Department of Chemistry, Purdue University,
West Lafayette, IN

Computational Quantum Chemistry

GK-12 Fellow/Lecturer Spring 2010
Tecumseh Middle High School, 8th Grade Science,
Purdue University,
West Lafayette, IN

The Graduate fellows in K-12 Education (GK-12)

Instructor/Tutor, Summer 2007-Summer 2009
Summer School on Computational Chemistry**,**
Jackson State University,
Jackson, MS

Computational Chemistry Problem Solving Sessions

Teaching Assistant/Instructor, Spring 2006
Department of Chemistry, Jackson State University,
Jackson, MS

General Chemistry Lab

Recitation Instructor, Spring 2006
Department of Chemistry, Jackson State University,
Jackson, MS

General Chemistry

Awards and Honors

Travel grant from the Purdue local section of the American Chemical Society, to attend The ACS National Meeting in Denver, CO. 2011

Grant for Community Service/Service Learning Projects – Project Title: "Hand-on Modeling of Molecular Structure and Chemical Bonding", Purdue University, West Lafayette, IN 2010

Best Oral Presentation, 2008-2009 Annual Meeting, Mississippi Academy of Sciences 2009

Best Graduate Poster in the 2009 Chemistry Day Poster Presentation, Jackson State University 2009

AAAS, Science Award for Excellence in Science for Students 2009

Certificate of Appreciation for Contribution as an Instructor/Tutor at 2008 Summer Institute on Quantum Chemistry, Jackson, MS 2008

Award for the Best Student Poster at
8th Southern School on Computational Chemistry, Jackson, MS 2008

First Place in Chemistry Challenge for January 2007,
Department of Chemistry, Jackson State University, Jackson, MS 2007

Award for the Best Student Poster at
7th Southern School on Computational Chemistry, Jackson, MS 2007

Bursary from Angela and Tony Fish Bequest,
Faraday Division, Royal Society of Chemistry, Nottingham, UK 2003

Service and Professional Memberships

AAAS, American Association for the Advancement of Science,
ACS, American Chemical Society
Sigma Xi, the Scientific Research Society
Executive committee member, 42nd Midwest Theoretical Chemistry Conference, Purdue University, 2010
Reviewer for Structural Chemistry

Professional Development

ACS Workshop for Prospective Chemistry Faculty August 20-21, 2010
ACS Boston, MA

Preparing Future Faculty Program Spring, 2010
Purdue University, the Graduate School

College Teaching Workshop Series Spring, 2010
Purdue University Center for Instructional Excellence

Career Development Workshop Series, Fall, 2009
Purdue University, the Graduate School

Qualifications

- **Electronic Structure and Molecular Mechanics Packages:**
  - Development: Q-Chem, GAMESS, PyQuante, WebMO.
  - Application: Gaussian, VASP, NWChem, CPMD, AIM2000, Amber, TINKER, COSMOtherm, GROMACS, LAMMPS, DALTON, TURBOMOLE.
- **Programming Languages:** C/C++, Visual C++, PHP, SQL, Perl, Java, Python, Pascal, Fortran, Assembler.
- **Databases:** MySQL, Microsoft SQL Server, Visual FoxPro.
- **Technologies:** GPU, CUDA, Win32 API, MFC, Sockets/Winsock, COM, OpenMP, Hardware Ports Programming.
- **Mathematical and Engineering Packages:** MATLAB, Mathematica, MathCAD, Statistica, Origin.
- **Web Development:** HTML, CSS, XML, PHP, AJAX, DOJO.
- **Scientific Graphics:** Avogadro, VMD, ChemOffice, Molden, Mercury, HyperChem, GaussView, MolDraw, *etc.*
- **Spectroscopy:** FTIR Spectroscopy, Spectroscopic Software: Opus, Omnic.

Publications

Journal Papers

1. Joanna C. Flick, **Dmytro Kosenkov**, C. David Sherril and Lyudmila V. Slipchenko "Accurate Prediction of Non-Covalent Interaction Energies with Effective Fragment Potential Method" *Journal of Physical Chemistry, 2011 (Submitted)*
2. James, William; Buchanan, Evan; Mueller, Christian; Dean, Jacob; **Kosenkov, Dmytro**; Slipchenko, Lyudmila; Guo, Li; Reidenbach, Andrew; Gellman, Samuel; Zwier, Timothy "Evolution of Amide Stacking in Larger γ-Peptides: Triamide H-Bonded Cycles" *J. Phys. Chem. A, 2011, 115 (47), 13783–13798*
3. Andrea Michalkova, Yana Kholod, **Dmytro Kosenkov**, Leonid Gorb, Jerzy Leszczynski "Origin of Life: Viability of Pyrite Pulled Metabolism in the "Iron-Sulfur World" Theory. Quantum Chemical Assessment" *Geochimica et Cosmochimica Acta 2011, 75 (7), 1933-1941*
4. **Dmytro Kosenkov**, Lyudmila V. Slipchenko Solvent "Solvent Effects on the Electronic Transitions of p-Nitroaniline: A QM/EFP Study" *J. Phys. Chem. A.* 2011, 115 (4), 392–401
5. Debashree Ghosh, **Dmytro Kosenkov**, Vitalii Vanovschi, Chris Williams, John Herbert, Mark Gordon, Michael Schmidt, Lyudmila Slipchenko and Anna I. Krylov "Non-covalent interactions in extended systems described by the Effective Fragment Potential method: Theory and application to nucleobase oligomers" *J. Phys. Chem. A.* 2010, 114 (48), 12739–12754
6. Tetyana Petrova, Igor Tarabara, Vitaliy Palchikov, Liliya Kasyan, **Dmytro Kosenkov**, Sergiy Okovytyy, Leonid Gorb, Svetlana Shishkina, Oleg Shishkin, and Jerzy Leszczynski "Ethanolysis of N-substituted

Norbornane Epoxyimides: Discovery of Diverse Pathways Depending on Substituent's Character, *Org. Biomol. Chem.* 2010, 8(9), 2142-2157

7. **Dmytro Kosenkov**, Yana A. Kholod, Leonid Gorb, Oleg V. Shishkin, Gulnara M. Kuramshina, Galina I. Dovbeshko, and Jerzy Leszczynski „Effect of a pH Change on the Conformational Stability of the Modified Nucleotide Queuosine Monophospate"*J. Phys. Chem. A.* 113 (33), 9386–9395, 2009
8. **Dmytro Kosenkov**, Yana Kholod, Leonid Gorb, Oleg Shishkin, Dmytro Hovorun, Michel Mons and Jerzy Leszczynski, "Kinetic simulation of Gas Phase Experiments: Cytosine and Guanine Tautomerization", *J. Phys. Chem B.* 2009 113 (17), 6140–6150
9. A. Michalkova, **D. Kosenkov**, L. Gorb, J. Leszczynski, "Thermodynamics and Kinetics of Intramolecular Water Assisted Proton Transfer in Na^+-1-Methylcytosine Water Complexes", *J. Phys. Chem B.* 112 (29), 8624-8633, 2008
10. Yana Kholod, **Dmytro Kosenkov**, Sergiy Okovytyy, Leonid Gorb, Mohammad Qasim, and Jerzy Leszczynski "CL-20 Photodecomposition: *Ab Initio* Foundations for Identification of Products", *Spectrochimica Acta A: Molecular and Biomolecular Spectroscopy* 71 (1), 230-237, 2008
11. **Dmytro Kosenkov**, Leonid Gorb, Oleg V. Shishkin, Jirí Šponer and Jerzy Leszczynski "Tautomeric Equlibrium, Stability and Hydrogen Bonding in 2□-Deoxyguanosine-Monophosphate Complexed with Mg^{2+}" *J. Phys. Chem B.* 2008, 112(1), 150-157
12. G.I. Dovbeshko, O.P. Gnatyuk, V.I. Chegel, Y.M. Shirshov, **D.V. Kosenkov**, E.A. Andreev, H.A. Tajmir-Riahi, P.M.Lytvyn "Gold and Colloidal Gold Surface Influence on DNA Conformational Change" *Semiconductor Physics, Quantum Electronics and Optoelectronics*, 2004, 7(3), 318-325.
13. Olena P. Repnytska, Galina I. Dovbeshko, Volodymyr P. Tryndiak, Igor M. Todor and **Dmitriy V. Kosenkov**, "Structural organisation of nucleic acids from tumour cells", *Faraday Discuss.* 126, 2004, 126, 61-76.

Chapters in Books

1. **Dmytro Kosenkov**, Yana Kholod, Leonid Gorb, And Jerzy Leszczynski, „Chapter 7 Evaluation of Proton Transfer in DNA Constituents: Development and Application of Ab Initio Based Reaction Kinetics", *Book: „Kinetics and Dynamics From Nano- to Bio-Scale" Series: „Challenges and Advances in Computational Chemistry and Physics"* Vol. 12, edited by Piotr Paneth, Agnieszka Dybala-Defratyka, 187-211, Springer Netherlands 2010,
2. G.I. Dovbeshko, O.P. Paschuk, O.M. Fesenko, V.I. Chegel, Yu.M. Shirshov, A.A. Nasarova, **D.V. Kosenkov**, "Biological Molecule Conformations Probed and Enhanced by Metal and Carbon Nanostructures: SEIRA, AFM and SPR Data", In Book*, Frontiers of Multifunctional Integrated Nanosystems*, Ed.: E. Buzaneva, P. Scharff, Kluwer Academic Publishers, 2004, 447-466
3. G. Dovbeshko, O. Repnytska, T. Pererva, A. Miruta, **D. Kosenkov**, "Vibrational spectroscopy and principal component analysis for conformational study of virus nucleic acids", *Proceedings of SPIE*. Ed. S.Sveshnikov, S.Kostyukevich, SPIE, Washington, 2004. Vol. 5507, 309-316
4. G.I. Dovbeshko, V.I. Chegel, O.P. Paschuk, Yu.M. Shirshov, A. Nasarova, **D. Kosenkov**, O. Fesenko "Biological Molecule Conformations Probed and Enhanced by Metal and Carbon Nanostructures". In Book, *Frontiers of Multifunctional Integrated Nanosystems*, Ed.: E. Buzaneva, P. Scharff, Kluwer Academic Publishers, 2003, 467-485

Selected Conference Presentations and Invited Talks

1. **Dmytro Kosenkov** and Lyudmila V. Slipchenko "Excitation Energy Transfer in Peridinin-Chlorophyll-Protein" *242nd ACS National Meeting & Exposition*, August 28 - September 1, 2011 Denver, CO
2. **Dmytro Kosenkov** and Lyudmila V. Slipchenko "First-Principles Based Modeling of Molecular Electronic Excitations in Biological Systems" *240th ACS National Meeting & Exposition*, 22-26 August, 2010 Boston, MA

3. **Dmytro Kosenkov** and Lyudmila V. Slipchenko "Electronic Excitations in Solution: First-Principles Based QM/MM Study" 240th ACS National Meeting & Exposition, 22-26 August, 2010 Boston, MA
4. **Dmytro Kosenkov** and Lyudmila V. Slipchenko, "A Combined Quantum Mechanics/Molecular Dynamics Simulation of Solvatochromic Shifts in Organic Chromophore p-Nitroaniline", *Gordon Research Conference on Atomic & Molecular Interactions*, 18-23 July, 2010, Colby-Sawyer College in New London, NH
5. **Dmytro Kosenkov** and Lyudmila V. Slipchenko, "Solvent Effects on the Electronic Transitions in p-Nitroaniline: A Combined Quantum Mechanics/Molecular Dynamics Simulation", *2010 Midwest Thermodynamics and Statistical Mechanics Conference*, June 2-3, 2010, University of Notre Dame, IN
6. **Dmytro Kosenkov** and Lyudmila V. Slipchenko, "QM/MM Simulations of UV Spectra of p-Nitroaniline in Organic Solvents", *Molecular Quantum Mechanics, an International Conference in Honor of Professor Henry F. Schaefer III*, May 24-29, 2010, University of California, Berkeley, CA
7. **Dmytro Kosenkov** and Lyudmila V. Slipchenko**,** "Solvent Effects on the Electronic Transitions in p-Nitroaniline: QM/MM Study" *42nd Midwest Theoretical Chemistry Conference*, May 20-22, 2010, *Purdue University*, West Lafayette, IN
8. **Dmytro Kosenkov**, Vitalii Vanovschi, Debashree Ghosh, Anna I. Krylov, Lyudmila V. Slipchenko "Implementation of the Effective Fragment Potential (EFP) method in Q-Chem" *Q-Chem Workshop*, 10-11 December, 2009, University of California, Berkeley, CA
9. **Dmytro Kosenkov**, Leonid Gorb, and Jerzy Leszczynski "Developing a Kinetic Model of Experiments on Isolated DNA Constituents" *Gordon Research Conference on Biological Molecules in the Gas Phase and in Solution*, 5-10 July, 2009 Tilton, NH
10. **Dmytro Kosenkov**, Leonid Gorb, and Jerzy Leszczynski "Kinetic Simulation of Gas Phase Experiments on Nucleobases" 237th ACS National Meeting & Exposition March 22-26, 2009 Salt Lake City, Utah
11. **Dmytro Kosenkov**, Yana Kholod, Leonid Gorb and Jerzy Leszczynski "Does Queuosine Nucleotide Exist in Zwitterionic Form?" , *"Mississippi Academy of Sciences, 2009 Annual Meeting"*, February 26-27, 2009, Olive Branch, MS
12. **Dmytro Kosenkov** "Nucleobases, Nucleotides, Nucleic Acids: Ab-Initio and Kinetic Simulations", *Prof. Mark Gordon Group Meeting, Department of Chemistry, Iowa State University,* July 2, 2008, Ames, Iowa
13. **Dmytro Kosenkov**, Yana Kholod, Leonid Gorb, Mohammad Qasim and Jerzy Leszczynski "Thermal Decomposition of RDX, HMX and CL-20: Kinetic Study", *"8th Southern School on Computational Chemistry"*, April 25-26, 2008**,** Jackson, MS
14. **Dmytro Kosenkov** "Why DNA is a Good Storage for Genetic Information: Quantum Chemical Investigation", *Theory Group Meeting, Department of Chemistry, University of Washington*, April 3, 2008
15. **Dmytro Kosenkov**, Yana Kholod, Leonid Gorb and Jerzy Leszczynski "Modeling of Space-Time Distribution of Multi-Component Reacting System. Implication for Prebiotic Evolution", *Book of Abstracts "16th Conference on Current Trends in Computational Chemistry"*, November 2-3, 2007 Jackson, Mississippi, USA
16. **Dmytro Kosenkov**, Leonid Gorb and Jerzy Leszczynski **'**Kinetic Simulation of Guanine Desorption in Gas-Phase Experiments' Book of Abstracts *"7th Southern School on Computational Chemistry"*, April 6-7, 2007**,** Jackson, Mississippi, USA, P67
17. **Dmytro Kosenkov**, Leonid Gorb, and Jerzy Leszczynski, 'Resonance-Enhanced Two-Photon Ionization Technique: Computer Simulation' Book of Abstracts *"15th Conference on Current Trends in Computational Chemistry"*, November 3-4, 2006**,** Jackson, Mississippi, USA, P88.
18. **Dmytro Kosenkov**, Leonid Gorb, Oleg V. Shishkin and Jerzy Leszczynski **'**Kinetic Model of Cytosine Bimolecular Tautomerization' Book of Abstracts *"6th Southern School on Computational Chemistry"*, April 7-8, 2006**,** Jackson, Mississippi, USA, P49.

19. **Dmytro Kosenkov**, Leonid Gorb, Yevgeniy Podolyan and Jerzy Leszczynski **'**Tautomeric Transitions in 2'-Deoxy-Guanosine-Monophosphate' Book of Abstracts *"14th Conference on Current Trends in Computational Chemistry"*, November 12-13, 2005**,** Jackson, Mississippi, USA, P90.
20. **Dmytro Kosenkov,** Galina I. Dovbeshko, Oleg V. Shishkin, Leond Gorb, Jerzy Leszczynski, Roman I. Zubatyuk "Molecular Structure of β-D-glucosylhydroxymethyluracil: a DFT Investigation" Book of Abstracts *"1st International Symposium on Methods and Applications of Computational Chemistry"*, 30 June – 1 July , 2005 Kharkiv, Ukraine, P44.