

# Dmytro Kosenkov

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## Education

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**Postdoctoral Research Associate**, Purdue University 2009  
Mentor: Prof. Lyudmila V. Slipchenko

**Ph.D. in Chemistry**, Jackson State University 2009  
Thesis: *“Thermodynamic and Kinetic Simulations on Biological Molecules in Gas Phase and in Solution: Evaporation, Isomerization, and Hydrogen Bonding”*  
Advisor: Prof. Jerzy Leszczynski

**M. S. in Physics**, National Taras Shevchenko University of Kyiv, Ukraine 2005

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

## Work Experience

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**Postdoctoral Research Associate**, Department of Chemistry, Purdue University 2009–Present

**Graduate Research Assistant**, Department of Chemistry, Jackson State University 2004–2009

**Teaching Assistant**, Department of Chemistry, Jackson State University, Jackson, MS 2006–2009

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

**Engineer**, Department of Physics of Biological Systems, Institute of Physics of National Academy of Sciences of Ukraine 2002–2005

## Awards and Honours

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Grant for Community Service/Service Learning Projects – Project Title: “Hand-on Modeling of Molecular Structure and Chemical Bonding”, Purdue University 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 During 2008 Summer Institute on Quantum Chemistry, Jackson, MS 2008

Second Award for The Best Student Poster at 8<sup>th</sup> Southern School on Computational Chemistry, Jackson, MS 2008

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

University, Jackson, MS

First Award for The Best Student Poster at 7<sup>th</sup> Southern School on Computational Chemistry, Jackson, MS 2007

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

## Professional Memberships

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**AAAS**, American Association for the Advancement of Science

**ACS**, American Chemical Society

**Sigma Xi**, The Scientific Research Society

## Research Interests

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The main field of my current research is computational chemistry. I work on several research projects:

- **Development QM/MM method based on Effective Potential (EFP) Model**
- **Dynamics of Electronic Excitations in DNA**
- **Application of EFP Model for Investigation of UV/Vis Spectra of Light-Sensitive Proteins**

I use *ab initio* quantum chemistry methods including first-principles molecular dynamics and chemical kinetics modeling for investigation of physical and chemical properties of organic solutions, biomolecules, carbon nanotubes and complex biological systems. Application of hybrid quantum mechanics/molecular mechanics methods allows me to simulate processes in solvents as well large biological molecules. I also develop software for electronic structure and chemical kinetics simulations to implement our models. My full research statement and current activities are available at <http://www.kosenkov.org>

## Technical Skills

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### **Electronic Structure and Molecular Mechanics Packages:**

Q-Chem (Development), Gaussian, VASP, NWChem, CPMD, AIM2000, Amber, TINKER, GAMESS, DALTON, TURBOMOLE, COSMOtherm, HyperChem

### **Scientific Graphics:**

VMD, ChemOffice, Molden, Mercury, HyperChem, GaussView, MolDraw, *etc.*

### **Mathematical and Engineering:**

MATLAB, MathCAD, Statistica, Origin, Mathematica

### **Infrared Spectroscopy Experimental:**

Fourier Transform Infrared (FTIR) Spectroscopy: Bruker IFS-45, IFS-60 instruments; Surface Enhanced Infrared Adsorption (SEIRA) Technique

### **Spectroscopic Software:**

Opus, Omnic

## IT Skills

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**Languages and Development Tools:** Visual C++, Pascal, Fortran, Assembler, PHP, SQL, Perl

**Databases:** MySQL, Microsoft SQL Server, Visual FoxPro

**Operating Systems:** Windows, Linux, UNIX, OS/2

**Web:** HTML, CSS, XML, XHTML, PHP, AJAX, DOJO

**Technologies:** Win32 API, MFC, Sockets/Winsock, COM, OpenMP, Hardware I/O Ports Programming

**Graphical Applications:** Corel Draw, Corel Photo-Paint, Adobe InDesign

## Publications

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### Journal Papers

1. Debashree Ghosh, **Dmytro Kosenkov**, Vitalii Vanovschi, Chris Williams, John Herbert, Mark Gordon, Michael Schmidt, Lyudmila V. Slipchenko and Anna I. Krylov, "Non-covalent interactions in large systems described by the effective fragment potential method" (*in preparation*)
2. **Dmytro Kosenkov**, and Jerzy Leszczynski „Combined ab initio/continuum mechanics approach for calculation of mechanical properties of polystyrene grafted nanotubes“ (*in preparation*)
3. **Dmytro Kosenkov**, Oleg V. Prezhdo, Bradley F. Habenicht, and Jerzy Leszczynski „First Principles Non-Adiabatic Molecular Dynamics Study of the DNA-SWCNT System“ (*in preparation*)
4. 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
5. **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 Monophosphate“ *J. Phys. Chem. A.* 113 (33), 9386–9395, 2009
6. **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
7. Anrea Michalkova, **Dmytro Kosenkov**, Leonid Gorb, Jerzy Leszczynski, "Thermodynamics and Kinetics of Intramolecular Water Assisted Proton Transfer in Na<sup>+</sup>-1-Methylcytosine Water Complexes", *J. Phys. Chem B.* 112 (29), 8624-8633, 2008
8. 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
9. **Dmytro Kosenkov**, Leonid Gorb, Oleg V. Shishkin, Jiri Šponer and Jerzy Leszczynski "Tautomeric Equilibrium, Stability and Hydrogen Bonding in 2'-Deoxyguanosine-Monophosphate Complexed with Mg<sup>2+</sup>" *J. Phys. Chem B.* 2008, 112(1), 150-157
10. 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.
11. 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, 2003, 126, 61-76.

### Articles in Books

1. **Dmytro Kosenkov**, Yana Kholod, Leonid Gorb, And Jerzy Leszczynski, „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, Spriger, (*in press*)
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**, 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
2. **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, New Hampshire
3. **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
  4. **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, Mississippi
  5. **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
  6. **Dmytro Kosenkov**, Yana Kholod, Leonid Gorb, Mohammad Qasim and Jerzy Leszczynski "Thermal Decomposition of RDX, HMX and CL-20: Kinetic Study", "8<sup>th</sup> Southern School on Computational Chemistry", April 25-26, 2008, Jackson, Mississippi, USA
  7. **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
  8. **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 "16<sup>th</sup> Conference on Current Trends in Computational Chemistry"*, November 2-3, 2007 Jackson, Mississippi, USA
  9. **Dmytro Kosenkov**, Leonid Gorb and Jerzy Leszczynski 'Kinetic Simulation of Guanine Desorption in Gas-Phase Experiments' Book of Abstracts "7<sup>th</sup> Southern School on Computational Chemistry", April 6-7, 2007, Jackson, Mississippi, USA, P67
  10. **Dmytro Kosenkov**, Leonid Gorb, and Jerzy Leszczynski, 'Resonance-Enhanced Two-Photon Ionization Technique: Computer Simulation' Book of Abstracts "15<sup>th</sup> Conference on Current Trends in Computational Chemistry", November 3-4, 2006, Jackson, Mississippi, USA, P88.
  11. **Dmytro Kosenkov**, Leonid Gorb, Oleg V. Shishkin and Jerzy Leszczynski 'Kinetic Model of Cytosine Bimolecular Tautomerization' Book of Abstracts "6<sup>th</sup> Southern School on Computational Chemistry", April 7-8, 2006, Jackson, Mississippi, USA, P49.
  12. **Dmytro Kosenkov**, Leonid Gorb, Yevgeniy Podolyan and Jerzy Leszczynski 'Tautomeric Transitions in 2'-Deoxy-Guanosine-Monophosphate' Book of Abstracts "14<sup>th</sup> Conference on Current Trends in Computational Chemistry", November 12-13, 2005, Jackson, Mississippi, USA, P90.
  13. **D.V. Kosenkov**, G. I. Dovbeshko, O. V. Shishkin, L. Gorb, J. Leszczynski, R. I. Zubatyuk "Molecular Structure of  $\beta$ -D-glucosylhydroxymethyluracil: a DFT Investigation" Book of Abstracts "1<sup>st</sup> International Symposium on Methods and Applications of Computational Chemistry", 30 June – 1 July, 2005 Kharkiv, Ukraine, P44.
  14. G. I. Dovbeshko, O. V. Shishkin, L. Gorb, J. Leszczynski, R. I. Zubatyuk and **D.V. Kosenkov** "Molecular Structure of Queuosine: A DFT Study" Book of Abstracts "13<sup>th</sup> Conference on Current Trends in Computational Chemistry", November 12-13, 2004 Jackson, Mississippi, USA, P47.
  15. G. I. Dovbeshko, O. V. Shishkin, L. Gorb, J. Leszczynski, R. I. Zubatyuk and **D.V. Kosenkov** "The role of H-bonding in formation of molecular structure of modified guanosine: DFT calculation and Bader's (AIM) analysis" Book of Abstracts "International Conference on Hydrogen Bonding Dedicated to Prof. Nikolay. D. Sokolov memory", October 6-10, 2004 Moscow, Klyaz'ma, Russia, P21.
  16. G.I. Dovbeshko, O.P. Gnatyuk, Yu.M. Shirshov, A.A. Nazarova, **D.V. Kosenkov**, E.D.Obraztsova "Conformations of Proteins Induced by Carbon Nanostructures: the SEIRA Data" Book of Abstracts "1<sup>st</sup> Ukrainian Conference on Biological and Medical Physics", September 20-23, 2004 Kharkov, Ukraine, P72.
  17. G. I. Dovbeshko, O. V. Shishkin, L. Gorb, J. Leszczynski, R. I. Zubatyuk and **D.V. Kosenkov** "Hypermodified Nucleotides Structure and Influence the Nucleic Acid Conformation" Book of Abstracts "1<sup>st</sup> Ukrainian Conference on Biological and Medical Physics", September 20-23, 2004 Kharkov, Ukraine, P37.
  18. G. Dovbeshko, A. Nazarova, **D. Kosenkov**, Ya. Shtogun , K. Ergen "SEIRA Study of serum albumin conformation under interaction with carbonaceous materials" Book of Abstracts "VII<sup>th</sup> International Conference on Molecular Spectroscopy". Wroclaw-Laddek Zdroj, 11-14.09.2003 Poland, P23.
  19. G. Dovbeshko, O. Repnytska, T. Pererva, A. Miruta, **D. Kosenkov** "Application of Vibrational Spectroscopy and Principal Component Analysis for Conformational Study of Virus Nucleic Acids", Book of Abstracts *Faraday Discussion 126*, RSC, Nottingham University, UK 2003.
  20. G. Dovbeshko, O. Repnytska, T. Pererva, A. Miruta, **D. Kosenkov** "Conformational Study of Virus Nucleic Acids: A SEIRA and Correlational Analysis Data", *Journal of Biomolecular Structure and Dynamics*, AdeninePress, NewYork, 2003, 20(20), P85