Dmytro Kosenkov

Office Address:
560 Oval Drive Box 134
West Lafayette, IN 47907-2084
USA

Tel: (765) 494-5489
Fax: (765) 494-5255

www.kosenkov.org

dkosenko@purdue.edu

Education

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*" Supervised by Prof. J. 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

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 Science 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

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 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

First Award for The Best Student Poster at 7th 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

AAAS, American Association for the Advancement of Science
ACS, American Chemical Society
Sigma Xi, The Scientific Research Society
MAS, Mississippi Academy of Sciences

Research Interests

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

- **Development of the general effective potential method (EFP) for QM/MM**
- **Investigation of Electronic Excitations in DNA Wrapped Carbon Nanotubes**
- **Mechanical Properties of Grafted Carbon Nanotubes**
- **Multiscale Simulation of Biological Neuronal Networks**
- **Biologically Inspired Methods of Computations**

I use *ab initio* quantum chemistry methods including first-principles molecular dynamics and chemical kinetics modeling for investigation of physical and chemical properties of biomolecules, nanotubes and complex biological systems.

Application of multiscale advanced physical and mathematical methods allows me to simulate processes under investigation. I also develop software to implement my models. My full research statement and current activities are available at **http://www.kosenkov.org**

Technical Skills

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

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

Journal Papers

1. **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
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. **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
5. 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
6. 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
7. **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
8. 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.
9. 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. 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
2. 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
3. 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", *"8th 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 "16th 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 *"7th 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
11. Ionization Technique: Computer Simulation' Book of Abstracts *"15th Conference on Current Trends in Computational Chemistry"*, November 3-4, 2006**,** Jackson, Mississippi, USA, P88.
12. **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.
13. **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.
14. **D.V. Kosenkov,** G. I. Dovbeshko, O. V. Shishkin, L. Gorb, J. Leszczynski, R. 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.
15. 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 *"13th Conference on Current Trends in Computational Chemistry"*, November 12-13, 2004 Jackson, Mississippi, USA, P47.
16. 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.
17. 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 "*1st Ukrainian Conference on Biological and Medical Physics"*, September 20-23, 2004 Kharkov,Ukraine, P72.
18. G. I. Dovbeshko, O. V. Shishkin, L. Gorb, J. Leszczynski, R. I. Zubatyuk and **D.V. Kosenkov** "Hypermodied Nucleotides Structure and Influence the Nucleic Acid Conformation" Book of Abstracts *"1st Ukrainian Conference on Biological and Medical Physics"*, September 20-23, 2004 Kharkov,Ukraine, P37.
19. G. Dovbeshko, A. Nazarova, **D. Kosenkov**, Ya. Shtogun , K. Ergen "SEIRA Study of serum albumin conformation under interaction with carbonaceous materials" Book of Abstracts *"VIIth International Conference on Molecular Spectroscopy"*. Wroclaw-Ladek Zdroj, 11-14.09.2003 Poland, P23.
20. 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.
21. 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

References

Available upon request