

Olexandr Isayev

Professional Preparation

In Progress	Ph.D. (expected in Spring 2008) Jackson State University, Department of Chemistry, Jackson, MS
2002	M.S. with the Highest Honor (Red Diploma) Dnepropetrovsk National University, Department of Chemistry, Ukraine
2001	B.Sc. with the Highest Honor Dnepropetrovsk National University, Department of Chemistry, Ukraine

Appointments

2002 – present	Graduate Research Assistant Computational Center for Molecular Structure and Interactions, Jackson State University, Jackson MS
Summer, 2006	Visiting Research Assistant Equipe de Chimie et Biochimie Théoriques, Université Henri Poincaré, Nancy, France
2004	Teaching Assistant Department of Chemistry, Jackson State University, Jackson MS
2000 – 2002	Research Associate Dnepropetrovsk National University, Department of Chemistry, Ukraine

Relevant Publications

1. O. Isayev, L. Gorb, M. Qasim, J. Leszczynski. An ab initio Molecular Dynamics Study of the Initial Chemical Events in Nitramines: CL-20 under Extreme Condition, 2008. (Submitted).
2. O. Isayev, A. Furmanchuk, L. Gorb, J. Leszczynski. Efficient and Accurate ab initio Prediction of Thermodynamic Parameters for Intermolecular Complexes. *Chem. Phys. Lett.* 2008, **451**, 147.
3. O. Isayev, L. Gorb, I. Zilberberg, J. Leszczynski. Electronic Structure and Bonding of {Fe(PhNO₂)₆}⁶⁺ complexes: A Density Functional Theory Study. *J. Phys. Chem. A*, 2007, **111**, 3571.
4. O. Isayev, L. Gorb, J. Leszczynski. Theoretical Calculations: Can Gibbs Free Energy for Intermolecular Complexes Be Predicted Efficiently and Accurately? *J. Comp. Chem.* 2007, **28**, 1598.
5. O. Isayev, B. Rasulev, L. Gorb, J. Leszczynski. Structure-Toxicity Relationships of Nitroaromatic Compounds. *Molecular Diversity*, 2006, **10**, 233.

Other Significant Publications

1. O. Isayev, A. Furmanchuk, O. Shishkin, L. Gorb, J. Leszczynski. Are Isolated Nucleic Acid Bases Really Planar? A Car-Parrinello Molecular Dynamics Study. *J. Phys. Chem. B*, 2007, **111**, 3476.
2. Zilberberg, M. Ilchenko, O. Isayev, L. Gorb, J. Leszczynski. Modeling the Gas-Phase Reduction of Nitrobenzene to Nitrosobenzene by Iron Monoxide: A Density Functional Theory Study. *J. Phys. Chem. A*, 2004, **108**, 4878.

Synergistic Activities

1. Research mentoring and teaching for CCMSI undergraduate summer schools (2003–2007), Jackson State University; Co-organizing and teaching for workshop on Molecular modeling of biomolecules (NSF Center for Workshops in the Chemical Sciences(CWCS) series), Jackson State University, April 2007. *Development and teaching of "Introduction to UNIX/Linux" class, research projects, and practical sessions for participants; formal and informal discussions with students.*
2. Member of local organizing committee for Conference on Current Trend of Computational Chemistry and Southern School on Computational Chemistry series of meetings, 2002–2007. *Responsibility for various aspects of the symposia, including development/support of online registration, and abstract submission systems; design and publication of the conference proceedings book, conference promotion; IT support on event locations.*
3. Teaching General Chemistry Lab (CHEML-141), Department of Chemistry, Jackson State University (2004).
4. System Administrator for Computational Center for Molecular Structure and Interactions, Jackson State University (2003–Present time). *Configuration/management of local computational clusters, workstations and servers; porting/tuning scientific codes on our platforms; development/management of department's web, mail and file servers. As part of collaboration with state and national supercomputing centers my efforts are devoted to benchmarking and enhancements computational chemistry codes on the new Cray X1E, XT3, and SGI Altix supercomputer platforms.*
5. Honor for Outstanding Academic Leadership, Jackson State University (2003). *Awarded annually, acknowledges best students who have outstanding academic records and a strong commitment to the education.*

Collaborators and Other Affiliations

Collaborators:

Mo, Quasim (US Army Engineer Research and Development Center (ERDC))

Zilberberg, Igor L. (Boreskov Institute of Catalysis, Russian Academy of Sciences, Russia)

Shishkin, Oleg V. (Institute for Single Crystals, National Academy of Science of Ukraine, Ukraine)

Ruiz-Lopez, Manuel (Université Henri Poincaré, Nancy, France)

Klueva, Natalia (Clark Atlanta University)

Ilchenko, Mykola (Institute of Cell Biology and Genetic Engineering, National Academy of Science of Ukraine, Ukraine)

Graduate Advisor:

Jerzy Leszczynski (Jackson State University)