

Curriculum Vitae

Yaroslava G. Yingling

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EDUCATION

- Penn State University**, University Park, PA, USA ▪ 2002
Ph.D. in Materials (with emphasis on Computational Materials Engineering)
Ph.D. minor in High Performance Computing Applications
Dissertation: "*Photochemical Processes in Laser Ablation of Organic Solids: Molecular Dynamics Study.*"
Advisor: Professor B. J. Garrison
- St.-Petersburg State Technical University**, St.-Petersburg, Russia ▪ 1996
B.S. in Computer Science and Engineering
Thesis: "*Numerical Control of Technical Systems by Application of the Law of Proportional-Integration*"
Advisor: Dr. V. D. Yarmiichuk

AWARDS AND HONORS

- National Institute of Health Postdoctoral Cancer Research Training Award ▪ 2004-2006
- Best Ph.D. Thesis Award from the Materials Research Institute at PSU ▪ 2003
- Braucher Fellowship for Graduate Student Research ▪ 2002
- Gordon Research Conference Travel Award ▪ 2002
- PSU Graduate Student Travel Award ▪ 2002
- Miller Graduate Student Research Award ▪ 2001
- St. Petersburg State Technical University merit-based stipend recipient ▪ 1991-1996

RESEARCH INTERESTS

- Interaction of radiation with biomolecules and biotissue with respect to cancer treatment and diagnostics;
- Multiscale molecular modeling from atomistic investigations of structure-function relationship of biomolecules to the development of advanced computational methods for large-scale biological materials and undergoing processes;
- Design and application of novel algorithms and high-performance computing techniques for modeling, simulations, data visualization and interpretation.

RESEARCH EXPERIENCE

- 2004-present** **Postdoctoral Research**, *Center for Cancer Research Nanobiology Program, National Cancer Institute, Frederick, MD.* (research advisor: Dr. Bruce A. Shapiro)
- Molecular modeling of RNA structure-function relationship.
- Structural and dynamical investigations of the human telomerase pseudoknot RNA domain;
 - Analyzed the effects of dyskeratosis congenita mutations on human telomerase;
 - Tertiary structure prediction and RNA folding;
 - Nanobiology studies of the design and development of functional nanodevices constructed from RNA molecules;
 - Investigated the mechanism of riboswitch sensor.
- 2002–2004** **Postdoctoral Research**, *Department of Chemistry, Penn State University, University Park, PA.* (research advisor: Dr. Barbara J. Garrison)
- Computational modeling of degradation and laser ablation of polymers.
- Developed a coarse-grain chemical reaction model simulating irradiation of polymeric materials via laser and/or atomic oxygen beam;
 - Applied this model to investigation of the degradation of PMMA in the space environment under synergetic effect of atomic oxygen bombardment and solar radiation;
 - Designed and performed calculations of UV laser irradiation of PMMA samples;
 - Investigated the primary mechanisms for onset of ablation in polymers.
- 1997-2002** **Doctoral Research**, *Department of Chemistry, Penn State University, University Park, PA.* (research advisor: Dr. Barbara J. Garrison)
- Multiscale modeling of photochemical and photothermal processes in organic solids.
- Developed a novel Coarse Grained Chemical Reaction Model (CGCRM) which permits the study of the effects of chemical reactions on large scale dynamic processes;
 - Applied the developed methodology to the molecular dynamics investigation of photochemical processes in laser ablation of organic materials;
 - Performed a comprehensive analysis of the role of photochemical reactions on laser ablation of organic materials;
 - Designed and performed calculations for investigation of the effect of volatility of solutes in laser ablation of bi-component organic materials;
 - Designed, implemented, and evaluated various algorithms on high-performance computers using parallel programming.
- 1994-1996** **Undergraduate Research**, *Department of Automation and Computer Science, St.-Petersburg State Technical University, St.-Petersburg, Russia.* (research advisor: Dr. Leonid V. Babko)
- Developed office-organization database for department;
 - Constructed programs for technical engineering design purposes;

- Participated in research management, experimental design, and review processes.

Summer 1995 Research Internship, *Department of Physics, St.-Petersburg National Military Space Academy, Russia.*

- Developed user-friendly interfaces for educational and organizational purposes;
- Constructed educational programs for physics laboratory;
- Participated in development of award winning educational software;
- Worked with databases and data processing.

TEACHING COMPETENCIES

Introductory and intermediate courses on materials science, physical chemistry, biophysics, biomaterials, bioinformatics, and biological macromolecules;

Advanced courses on computational materials, biomaterials science and engineering, and molecular modeling.

TEACHING EXPERIENCE

Supervised and directed research projects done by undergraduate and graduate students at Penn State University and at the National Cancer Institute that resulted in publications and presentations at scientific meetings.

At Penn State University, University Park, PA:

Spring 2000 Teaching Assistant – *Computer Simulations for Physical Scientists (Graduate Course).*

Prepared and presented lectures on High Performance Computing Applications, created and graded homework assignments, graded exams, held office hours, tutored students on demand.

Fall 1997 Teaching Assistant – *Experimental Physical Chemistry Lab*

Prepared short lectures, demonstrated experiments, taught laboratory sessions, graded all written work including lab reports, quizzes, final exams, and tutored students weekly.

1997- 2000 Grader – Graded and supervised exams for Organic Chemistry, Physical Chemistry, and Quantum Chemistry courses.

At St.-Petersburg State Technical University, St.-Petersburg, Russia:

1994-1996 Physics and Math Tutor – Tutored physics and math for freshman and sophomore technical majors; prepared high school students for University physics and math entrance exams.

PUBLICATIONS

1. **Y. G. Yingling**, L. V. Zhigilei, B. J. Garrison, A. Koubenakis, J. Labrakis, S. Georgiou, Laser Ablation of Bi-component Systems: A Probe of Molecular Ejection Mechanisms, *Appl. Phys. Lett.* **78** (2001) 1631-1633.

2. **Y. G. Yingling**, L. V. Zhigilei, B. J. Garrison, Photochemical Fragmentation Processes in Laser Ablation of Organic Solids, *Nucl. Instrum. Methods Phys. Research B* **180** (2001) 171-175.
3. **Y. G. Yingling**, L. V. Zhigilei, B. J. Garrison, The Role of the Photochemical Fragmentation in Laser Ablation, *J. Photochemistry and Photobiology A: Chemistry* **145** (2001) 173-181.
4. **Y. G. Yingling**, B. J. Garrison, Photochemical induced effects in material ejection in laser ablation, *Chem. Phys. Lett.* **364** (2002) 237-243.
5. B. J. Garrison, A. Delcorte, L. V. Zhigilei, T. E. Itina, K. D. Krantzman, **Y. G. Yingling**, C. M. McQuaw, E. J. Smiley, N. Winograd, Big Molecule Ejection - SIMS vs. MALDI, *Appl. Surf. Sci.* **69-71** (2003) 203-204.
6. L. V. Zhigilei, E. Leveugle, B. J. Garrison, **Y. G. Yingling**, M. I. Zeifman, Computer Simulations of Laser Ablation of Molecular Substrates, *Chem. Reviews* **103** (2003) 321-348.
7. L. V. Zhigilei, **Y. G. Yingling**, T. E. Itina, T. A. Schoolcraft, B. J. Garrison, MD Simulations of MALDesorption - Connections to Experiment, *Int. J. Mass Spectrom.* **226** (2003) 85-106.
8. **Y. G. Yingling**, B. J. Garrison, Photochemical Ablation of Organic Solids, *Nucl. Instrum. Methods Phys. Research B* **203** (2003) 188-194.
9. **Y. G. Yingling**, B. J. Garrison, Coarse Grained Chemical Reaction Model, Feature Article in *J. Phys. Chem. B* **108** (2004) 1815-1821.
10. **Y. G. Yingling**, P. F. Conforti, B. J. Garrison, Theoretical Investigation of Laser Pulse Width Dependence in Thermal Confinement Regime, *Appl. Phys. A* **79** (2004) 757-759.
11. **Y. G. Yingling**, B. J. Garrison, Coarse-Grained Model of Interaction of Light with Polymeric Material: Onset of Ablation, *J. Phys. Chem. B* **109** (2005) 16482-16489.
12. **Y. G. Yingling**, B. A. Shapiro, Dynamic Behavior of the Telomerase RNA Hairpin Structure and Its Relationship to Dyskeratosis Congenita, *Journal of Molecular Biology* **348** (2005) 27-42.
13. W. A. Hastings, **Y. G. Yingling**, G. S. Chirikjian, B. A. Shapiro, Structural and Dynamical Classification of RNA Single-Base Bulges for Nanostructure Design, to appear in *J. of Computational and Theoretical Nanoscience*, (2005).

Manuscripts submitted:

14. P. F. Conforti, **Y. G. Yingling**, B. J. Garrison, Computational Studies of Ultraviolet Ablation of Poly(Methyl MethAcrylate), *Journal of Physics: Conference Series*, submitted (2005).
15. **Y. G. Yingling**, B. A. Shapiro, The Determination of the Wild-type Telomerase RNA Pseudoknot Structure and the Pivotal Role of a Bulge in its Formation, submitted (2005).
16. **Y. G. Yingling**, B. A. Shapiro, The Effects of Dyskeratosis Congenita Mutations on Structure and Dynamics of the Telomerase RNA Pseudoknot Domain (2005), in preparation.

 PROFESSIONAL AND COMMUNITY ACTIVITIES

- Judge for Pennsylvania Junior Academy of Science▪ 1998-2001
 - PSU Graduate Research Exhibition Judge▪ 2002-2003
 - Frederick Skating Club Publicity Officer▪ 2004-present
 - Referee for Applied Physics Letters, Applied Surface Science
 - Member of American Physical Society, American Chemical Society
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 PRESENTATIONS

- Molecular Dynamics Model for Laser Ablation of Organic Solids, Y. G. Zhiltsova (Yingling), P. B. S. Kodali, L. V. Zhigilei, B. J. Garrison, *Graduate Research Exhibition*, Penn State University, University Park, PA, March 24, 1997, **poster**.
- Molecular Dynamics Simulation Study of Laser Ablation of Chlorobenzene, Y. G. Zhiltsova (Yingling), L. V. Zhigilei, B. J. Garrison, *APS Centennial Meeting*, Atlanta, Georgia, March 20-26, 1999, **poster**.
- Influence of analyte volatility on molecular ejection processes in laser ablation, Y. G. Yingling, L. V. Zhigilei, B. J. Garrison, A. Koubenakis, S. Georgiou, *48th ASMS Conference*, Long Beach, CA, June 11-15, 2000, **talk**.
- Ejection mechanisms of analytes in the UV ablation of model molecular solids: implications for MALDI, A. Koubenakis, J. Labrakis, S. Georgiou, Y. G. Yingling, L. V. Zhigilei, B. J. Garrison, *GRC on Laser Interactions with Materials*, NH, June 11-16, 2000, **poster**.
- Ejection Efficiency of Analytes of Different Volatility in Laser Ablation of Organic Solids, Y. G. Yingling, L. V. Zhigilei, B. J. Garrison, *5th Int. Conf. on Computer Simulation of Radiation Effects in Solids (COSIRES'2000)*, Penn State University, University Park, PA, July 24-28, 2000, **talk**.
- Photochemical Processes in Laser Ablation of Organic Solids, Y. G. Yingling, B. J. Garrison, *6th Int. Conf. on Computer Simulation of Radiation Effects in Solids (COSIRES'2002)*, Dresden, Germany, June 23-27, 2002, **invited talk**.
- Photochemical Processes in Laser Ablation. Molecular Dynamics Study, Y. G. Yingling, *Phys. Chem. Seminar*, Penn State University, University Park, PA, May 17, 2002, **seminar**.
- The influence of photochemical processes on laser ablation mechanism. Molecular Dynamics Study, Y. G. Yingling, B. J. Garrison, *Gordon Research Conference on Laser Interactions with Materials*, NH, June 21-26, 2002, **poster**.
- Mesoscopic Computer Modeling of Laser Ablation, B. J. Garrison, Y. G. Yingling, L. V. Zhigilei, *225th ACS National Meeting*, New Orleans, LA, March 23-27, 2003, invited talk.
- Photochemical Processes in Laser Ablation of Organic Materials. Molecular Dynamics Study, Y. G. Yingling, B. J. Garrison, *Second Annual Materials Day*, Penn State University, University Park, PA, April 15, 2003, **poster**.
- Mesoscale Modeling of Laser Irradiation of Organic Materials, Y. G. Yingling, *National Cancer Institute Center for Cancer Research*, Frederick, MD, May 15, 2003, **seminar**.
- Application of Coarse Grain Chemical Reaction Model to Degradation of PMMA under LEO conditions, Y. G. Yingling, M. Medvedeva, B. J. Garrison, *Materials*

Degradation/Passivation in the Space Environment annual review meeting, University of Pittsburgh, Pittsburgh, PA, August 19-20, 2003, **poster**.

- Photochemical Processes in Laser Ablation of Organic Materials, Y. G. Yingling, B. J. Garrison, *International Conference on Laser Ablation (COLA'03)*, Hersonissos, Crete, Greece, October 5-10, 2003, **invited talk**.
- Photochemical Processes in Laser Ablation of Organic Materials, Y.G. Yingling, B.J. Garrison, APS Meeting, Montreal, March 24, 2004, **invited talk**.
- Mesoscale Modeling of Chemical Reactions in Laser Ablation of Polymers, Y.G. Yingling, B.J. Garrison, APS Meeting, Montreal, March 24, 2004, **talk**. Molecular Dynamics Simulations of Laser Ablation, P. F. Conforti, Y.G. Yingling, B. J. Garrison, *228th ACS National Meeting, Philadelphia*, PA, August 22-26, 2004, **poster**.
- Theoretical studies of Laser Ablation of Poly(methyl methacrylate), P.F. Conforti, T. Nedelia, Y.G. Yingling, B. J. Garrison, *Gordon Research Conference on Laser Interactions with Materials*, NH, July 2004, **poster**.
- UV radiation and O atom bombardment of Poly(methyl methacrylate), P.F. Conforti, T. Nedelia, Y.G. Yingling, B. J. Garrison, *Materials Degradation/Passivation in the Space Environment annual review meeting*, January 2005, **poster**.
- Molecular Dynamics Study of Telomerase RNA and the effects of the Dyskeratosis Congenita mutations, Y. G. Yingling, B. A. Shapiro, *National Cancer Institute Spring Research Festival*, NCI-Frederick, May 2005, **poster**
- Exploration of Wild-Type Telomerase RNA Structure via Molecular Dynamics Simulations, Y. G. Yingling, B. A. Shapiro, NIH Research festival, Bethesda, MD, October 18-21, 2005, **poster**.

COMPUTER COMPETENCY

Computational science

- Molecular Dynamics/Mechanics methods
- Statistical Simulation Methods (various Monte Carlo methods)
- Finite Difference Time Domain (FDTD) method for electromagnetics
- Finite Elements method
- Finite Difference methods

Scientific Computing

- Design and implementation of numerical methods
- Analysis and visualization of large data sets
- Statistical modeling
- Numerical linear and vector algebra, differential equations
- Parallel and vector computers (Cray T3E, SGI Origin, IBM SP/2, Altix)
- Parallel programming via OMP, SMP, MPI
- Performance analysis and modeling
- Optimization methods and algorithms

Information technology

- Fortran77/90/95, C/C++, Pascal/Turbo-Pascal, Assemblers, Basic, Java
- Molecular modeling software (Amber, NAMD, CHARMM, Materials Studio, InsightII, Gaussian98)
- Scientific software (Mathematica, Tecplot, Matlab)
- Applications and system programming (Unix, DOS, MS Windows, AIX)
- Web-based systems (XML, HTML, CSS)

REFERENCES

- (1) **Dr. Barbara J. Garrison**, Shapiro Professor of Chemistry
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Chemistry Department,
Pennsylvania State University,
University Park, PA, 16802
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- (2) **Dr. Bruce A. Shapiro**, Principal Investigator
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Center for Cancer Research Nanobiology Program,
National Cancer Institute, NCI-Frederick,
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- (3) **Dr. Ruth Nussinov**, Professor of Human Genetics and Molecular Medicine and Principal Investigator
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- (4) **Dr. Leonid V. Zhigilei**, Associate Professor of Material Science and Engineering
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Department of Materials Science and Engineering,
University of Virginia,
Charlottesville, VA 22904
Email: lz2n@virginia.edu
Phone: 434-243-3582
- (5) **Dr. Tatiana E. Itina**, Research Scientist
Address: Laboratory of Lasers, Plasmas, and Photonic Processing (LP3 CNRS),
Faculte des Sciences de Luminy,
Case 917, 13288,
Marseille, Cedex 9, France
E-mail: itina@lp3.univ-mrs.fr
Phone: 33-4-91-82-92-83
- (6) **Dr. Hugo M. Martinez**, Emeritus Professor of Biophysics
Address: Department of Biochemistry and Biophysics,
University of California at San Francisco
San Francisco, CA 94143
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