Curriculum Vitae

Contact Information

Home Address	Ehm-Welk-Str. 24 Bargeshagen, 18211, Germany
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Work Address	Institut für Physik, Universität Rostock, Albert Einstein Straße 23-24, 18059 Rostock
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Personal Details

Name	Sergey Dmitrievich Ivanov
Date of Birth	5th September 1976
Nationality	Russian

Research interests

Quantum dynamics, path integrals, semiclassical methods

(ab initio) Molecular Dynamics, Monte Carlo methods, QM/MM techniques

Quasiclassical dynamics (Centroid MD, Ring polymer MD)

Linear and non-linear vibrational spectroscopy

Free energy methods

System-bath partitioning approaches, Generalized Langevin equation

Complex many-body systems towards condensed phase, biomolecules

Massively parallel computing, GPU computing

I'm particularly interested in method testing and development

Postdoctoral experience

April 2006 – October 2011 Wissenschaftlicher Mitarbeiter, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany

November 2011 – present Senior researcher, Quantum dynamics group, Institute of Physics, Rostock University, Rostock, Germany

Education (in reversed order)

1. Ph.D., Physical Chemistry, Stockholm University, Stockholm, Sweden. September, 2005. Dissertation: "Path Integral studies of quantum systems at finite temperatures" (in English). Advisor: Prof. Alexander Lyubartsev

2. Master of Science, Physics, Degree with Honors. Saint-Petersburg State University, Physics Faculty, Saint-Petersburg, Russia. November, 1999.
Thesis: "Thermodynamics of the quantum gas in an arbitrary external field: exact

expressions and numerical treatment" (in Russian).
Supervisor Prof. P. N. Vorontsov-Velyaminov

3. Bachelor of Science, Physics. Degree with Honors. Saint-Petersburg State University, Physics Faculty, Saint-Petersburg, Russia. June, 1997.
Thesis: "Monte Carlo method in Expanded ensemble for computation of free energies of lattice polymer systems" (in Russian).
Supervisor Prof. P. N. Vorontsov-Velyaminov

4. Graduated from the special physical-mathematical School No. 239 in Saint-Petersburg in June 1993.

Awards

1. The winner of the personal grants' competition in the field of fundamental research, held by the government of Saint-Petersburg, for students and young scientists of Saint-Petersburg in 1998, 1999, 2000 years.

2. "Soros graduate student" in 1999.

3. "Soros Ph.D. student" in 2000.

Skills

Languages Russian (native), English (fluent), German

Programming FORTRAN, C, C++, Pascal, tcl, Linux shell–scripting, MPI/OpenMP, CUDA

Platforms Experience in running large scale simulations on BlueGene, SGI Altix 4700, and various Linux clusters

Program packages Coding: CPMD (in FORTRAN); wrote CPMD TestSuite (with Gerald Mathias)
Using: CPMD, CP2K, Turbomole, Gaussian, Gromacs

Personal grants

Ongoing DFG grant IV 171/2-1 (Eigene Stelle) from May 2015 for two years.

Students

1. Marc Dämgen, Bachelor Thesis "Analyzing Quantum Effects of Protonated Water Networks in Bacteriorhodopsin", September 2009 (co-supervised, under the supervision of Prof. Dominik Marx)

2. Theodros Zelleke, Spezialisierung "Path Integral QM/MM Metadynamics: choice of a suitable enzymatic reaction", July 2010 (co-supervised, under the supervision of Prof. Dominik Marx)

3. Theodros Zelleke, Master Thesis "Computer simulation of Methylamine Dehydrogenase", February 2011 (co-supervised, under the supervision of Prof. Dominik Marx)

4. Alexander Witt, Ph. D. Thesis "Quantum Simulation of Molecular Systems: Dynamics and IR Spectroscopy of CH_5^+, its Isotopologues, and Microsolvated Species" December 2010, (co-supervised, under the supervision of Prof. Dominik Marx)

5. Tobias Zentel, Master Thesis "(Non)-linear spectroscopy Based on Classical Trajectories"
September 2012, (co-supervised, under the supervision of Prof. Oliver Kühn)

6. Fabian Gottwald, Bachelor Thesis "Why does classical molecular dynamics yield quantum–mechanical infrared spectra?"
September 2012, (co-supervised, under the supervision of Prof. Oliver Kühn)

7. Sven Karsten, Bachelor Thesis "Towards precise benchmarks for the infrared spectra provided by quasi-classical simulations"
November 2012, (co-supervised, under the supervision of Prof. Oliver Kühn)

8. Julius Zimmermann, Bachelor Thesis "Treating Coulomb Singularities by Means of Bead Fourier Path Integral Techniques"
August 2014, (co-supervised, under the supervision of Prof. Oliver Kühn)

9. Fabian Gottwald, Master Thesis "Vibrational Spectroscopy via Generalized Langevin Dynamics: Applicability and Beyond"
September 2014, (co-supervised, under the supervision of Prof. Oliver Kühn)

10. Sven Karsten, Master Thesis "Infrared Spectroscopy via Path Integral Techniques"
October 2014, (co-supervised, under the supervision of Prof. Oliver Kühn)

11. Chris Rehhagen, Bachelor Thesis "Determining the free energies and reaction mechanisms via accelerated molecular dynamics"
November 2014, (co-supervised, under the supervision of Prof. Oliver Kühn)

12. Till Köster, Bachelor Thesis "Sampling the Wigner function for semiclassical initial value representation methods"
September 2015, (co-supervised, under the supervision of Prof. Oliver Kühn)

Publications (in chronological order)

1999 *1* P. N. Vorontsov-Velyaminov, D. A. Ivanov, S. D. Ivanov and A. V. Broukhno, *Expanded ensemble Monte Carlo calculations of free energy for closed, stretched and confined lattice polymers* Colloids and Surfaces A, **148**, 171–177 (1999)

2 P. N. Vorontsov-Velyaminov, S. D. Ivanov, R. I. Gorbunov, *Quantum gas in an external field: Exact grand canonical expressions and numerical treatment*, Phys. Rev. E, **58**, 168–176, (1999)

3 P. N. Vorontsov-Velyaminov, R. I. Gorbunov, S. D. Ivanov, *Bead-Fourier Path Integral Monte Carlo method applied to systems of identical particles*, Comput. Phys. Commun., **121–122**, 64–66, (1999)

2000 *4* P. N. Vorontsov-Velyaminov, R. I. Gorbunov, S. D. Ivanov, *Trapped mesoscopic quantum gas in a magnetic field*, J. Phys. A, **33**, 1857–1871, (2000)

2003 *5* S. D. Ivanov, A. P. Lyubartsev, and A. Laaksonen, *Bead-Fourier Path Integral molecular dynamics*, Phys. Rev. E, **67**, 066710, (2003)

2005 *6* S. D. Ivanov and A. P. Lyubartsev, *Simulations of one- and two-electron systems by Bead-Fourier Path Integral molecular dynamics*, J. Chem. Phys., **123**, 034105, (2005)

2006 *7* S. D. Ivanov and A. P. Lyubartsev, *Bead-Fourier Path Integral molecular dynamics for identical particles*, Proceedings of the 8th International Conference "Path Integrals. From Quantum Information to Cosmology". (2006)

2008 *8* A. Witt, S. D. Ivanov, H. Forbert, and D. Marx *Microsolvation of Protonated Methane: Structures and Energetics of* $CH_5^+(H_2)_n$, J. Phys. Chem. A, **112**, 12510–12517 (2008)

2009 *9* A. Witt, S. D. Ivanov, M. Shiga, H. Forbert, and D. Marx *On applicability of Centroid and Ring Polymer molecular dynamics for simulating IR spectra*, J. Chem. Phys., **130**, 194510 (2009)

10 A. Witt, S. D. Ivanov, and D. Marx *Ab Initio Path Integral Simulations of Floppy Molecular Systems* in High Performance Computing in Science and Engineering, Garching/Munich, 675–686, 2009

2010 *11* S. D. Ivanov, A. Witt, M. Shiga, and D. Marx *On Artificial Frequency Shifts in Infrared Spectra obtained from Centroid Molecular Dynamics: Quantum Liquid Water*, J. Chem. Phys., **132**, 031101 (2010)

12 S. D. Ivanov, O. Asvany, A. Witt, E. Hugo, G. Mathias, B. Redlich, D. Marx, and S. Schlemmer *Quantum-induced symmetry breaking explains IR spectra of* CH_5^+ *isotopologues*, Nature Chemistry, **2**, 298–302 (2010)

2011 *13* A. Witt, S. D. Ivanov, G. Mathias, and D. Marx *Quantum Molecular Dynamics Calculations of Ultrafast Time Scales and Infrared Spectra of Protonated Methane: Quantifying Isotope-Specific Lifetimes*, J. Phys. Chem. Lett., **2**, 1377–1381 (2011)

2012 *14* G. Mathias, S. D. Ivanov, A. Witt, M. D. Baer, and D. Marx *Infrared Spectroscopy of Fluxional Molecules from (ab Initio) Molecular Dynamics:*

Resolving Large-Amplitude Motion, Multiple Conformations, and Permutational Symmetries, J. Chem. Theory Comput., 2012, **8** (1), 224–234.

2013 *15* A. Witt, S. D. Ivanov, D. Marx
Microsolvation-Induced Quantum Localization in Protonated Methane
Phys. Rev. Lett. **110**, 083003 (2013)

16 S. D. Ivanov, A. Witt, D. Marx
Theoretical Spectroscopy from Molecular Dynamics: Theory and Application to CH_5^+ and its Isotopologues, PhysChemChemPhys, **15**, 10270–99 (2013)

2015 *17* M. Schröter, S. D. Ivanov, J. Schulze, S. P. Polyutov, Y. Yan, T. Pullerits, O. Kühn
Exciton-vibrational coupling in the dynamics and spectroscopy of Frenkel excitons in molecular aggregates, Physics Reports **567**, 1-78

18 F. Gottwald, S. D. Ivanov*, O. Kühn
On the Applicability of the Caldeira-Leggett Model to Vibrational Spectroscopy in Solution, J. Phys. Chem. Lett., **6** (14), 2722-2727

19 F. Gottwald, S. Karsten, S. D. Ivanov*, O. Kühn
Parametrizing linear generalized Langevin dynamics from explicit molecular dynamics simulations, J. Chem. Phys., **142** (24), 244110

20 S. D. Ivanov, I. M. Grant, D. Marx
Quantum free energy landscapes from ab initio path integral metadynamics: Double proton transfer in the formic acid dimer is concerted but not correlated, J. Chem. Phys. **143**, 124304

2016 *17* F. Gottwald, S. D. Ivanov, O. Kühn
Vibrational spectroscopy via the Caldeira-Leggett model with anharmonic system potentials, arXiv:1601.04470 [physics.chem-ph]

Teaching Experience (in chronological order)

4 weeks Teaching assistant during the Masters program at St.-Petersburg State University (in Russian).

8 months full time Teaching assistant during the Ph.D. studentship at Stockholm University. (in English)

WS 2006/2007 Teaching assistant in the advanced course "Dynamics and Simulation" of Dr. Nikos Doltsinis (in English)

WS 2007/2008 Teaching assistant in the advanced course "Dynamics and Simulation" of Prof. Dominik Marx (in English)

WS 2008/2009 Teaching assistant in the advanced course "Dynamics and Simulation" of Prof. Dominik Marx (in English)

WS 2010/2011 Teaching assistant in the advanced course "Dynamics and Simulation" of Dr. Jörg Behler (in English)

WS 2011/2012 Teaching assistant in the advanced course "Molecular Physics" of Prof. Oliver Kühn (in English)

SS 2012 Teaching assistant in the advanced course "Spectroscopy and non-linear optics" of Prof. Oliver Kühn (in English)

SS 2012 Teaching assistant in the basic course "Theor. Phys. II (Mechanik)" of Prof. Oliver Kühn (in German)

WS 2012/2013	Teaching assistant in the advanced course "Molecular Physics" of Prof. Oliver Kühn (in English)
SS 2013	Teaching assistant in the advanced course "Spectroscopy and non-linear optics" of Prof. Oliver Kühn (in English)
SS 2013	Teaching assistant in the basic course "Theor. Phys. II (Mechanik)" of Prof. Stephan Scheel (in German)
SS 2013	Supervision of the project "Path integral molecular dynamics" within the advanced laboratory course for master students (Forschungpraktikum-III, 3 SWS, in English)
WS 2013/2014	Lecturer in the advanced course: "Advanced Theoretical Physics" within the international master programme (in English)
WS 2013/2014	Supervision of computer laboratory for the advanced course: "Advanced Theoretical Physics" (in English)
SS 2014	Teaching assistant in the advanced course "Spectroscopy and non-linear optics" of Prof. Oliver Kühn (English/German)
SS 2014	Supervision of the project "Path integral molecular dynamics" within the advanced laboratory course for master students (Forschungpraktikum-III, 3 SWS, in English)
WS 2014/2015	Lecturer in the advanced course: "Advanced Theoretical Physics" within the international master programme (in English)
WS 2014/2015	Supervision of computer laboratory for the advanced course: "Advanced Theoretical Physics" (in English)
SS 2015	Supervision of the project "Path integral molecular dynamics" within the advanced laboratory course for master students (Forschungpraktikum-III, 3 SWS, in English)
WS 2015/2016	Lecturer in the advanced course "Simulation methods of molecular Biophysics" (3 SWS in English)
SS 2016	Supervision of the project "Metadynamics" within the advanced laboratory course for master students (Forschungpraktikum-III, 3 SWS, in English)

Rostock, March 10, 2016