



Curriculum Vitae

Personal Information

First name(s) / Surname(s)

Khatuna Kakhiani

Mailing Address(es)

Faculty of Exact and Natural Sciences, Tbilisi State University, 3 Chavchavadze Ave., 0128 Tbilisi, Georgia

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Nationality

Georgian

Occupational field

Head Specialist of Educational Process Administration and Scientific Research

Dates

13.03.2009 - Present

Main Activities and Responsibilities

- Supervising faculty master's programs; students
- Financing master students through fellowship competitions
- Leading scientific seminars for the chemistry department
- Lead a summer science academy for students interested in exact and natural sciences, organized and managed the teaching staff and academy program
- Lead the kids-university at the Physics department
- Lead collaboration activities with TU Muenchen, other internationalization activities within the faculty
- An ambassador of DAAD within the faculty
- Providing consultations regarding the scientific foundation and patenting

SUMMARY OF QUALIFICATIONS

- Expert knowledge in theoretical chemical kinetics, including statistical, classical trajectory, and ab initio electronic structure methods
- Experience with atomistic simulation methods
- Strong background in theoretical and combustion chemistry
- Experience with gas-phase, "on the fly" direct dynamics and utilization of high-performance massively parallel computing
- Experience in development and validation of first-principles theoretical calculations

Relevant experience in generating detailed reaction mechanisms of the chemistry of extreme environments and for making quantitative predictions of elementary rate coefficients

Name and Address of Employer	Faculty of Exact and Natural Sciences, Tbilisi State University, Georgia
Type of Business or Sector	University, Research, Education
Dates	02.01.2007 – 6.03.2009
Occupation or Position Held	Postdoctoral Research Associate
Main Activities and Responsibilities	<ul style="list-style-type: none"> • Simulation of direct dynamics of cyclohexane isomerisation and the dynamics of the twist-boat intermediate at an atomistic, microscopic level using direct classical molecular dynamics and quantum mechanical methods (Venus-NWchem) • Development of source code for conformational analysis • Development of source code for molecular mechanic potential (MM3) in the classical dynamics program package Venus (relevant for QM/MM applications) • electronic structure calculations
Name and Address of Employer	Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, USA
Type of Business or Sector	University, Research
Dates	13.09.2004 – 21.12.2006
Occupation or Position Held	Postdoctoral Research Associate
Main Activities and Responsibilities	<ul style="list-style-type: none"> • Calculation of the CH₂ + H recombination rate constant using the new global Potential Energy Surface (PES) for CH₃ by means of various methods, including classical trajectory calculations and statistical theories such as Variational Transition State Theory (VTST), Flexible Transition State Theory (FTST), and Statistical Adiabatic Channel Model (SACM) • Coding of parts of various program packages, such as Variflex and Polyrate, as well as the development of new program ESACM
Name and Address of Employer	Chemical Dynamics in the Gas Phase Group, Argonne National Laboratory, USA
Type of Business or Sector	Research Institution
Dates	01.08.1999 – 10.09.2004
Occupation or Position Held	Research and Teaching Assistant
Main Activities and Responsibilities	<ul style="list-style-type: none"> • Investigation of the influence of rotation on the pressure and temperature dependence of rate constants and the branching ratios of multi-channel unimolecular reactions • Development of a computer program to solve one and two-dimensional Master Equations and RRKM method (FORTRAN 90) • Study of thermal decomposition of methyl radical, allyl radical, toluene, formaldehyde, and methane by means of the Statistical Adiabatic Channel Model (SACM) and Master Equation analysis • Tutor for the courses: "Reaction Kinetics" and "Physical Chemistry". Preparation of lecture and delivery of exercise materials in both beginner and advanced classes
Name and Address of Employer	Chair of Molecular Physical Chemistry, University of Karlsruhe (TH), Germany
Type of Business or Sector	University, Research
Dates	1990 - 2000
Occupation or Position Held	Research Scientist

Main Activities and Responsibilities Study of the biologically active complex compounds of transition metals with Pyridine Carbon Acids by means of semiempirical and ab initio quantum mechanical as well as IR/RAMAN spectroscopic methods

Name and Address of Employer Institute of Inorganic Chemistry and Electrochemistry, Georgian Academy of Sciences, Georgia
 Type of Business or Sector Research Institute

Education and Training

Date 2004
 Title of Qualification Awarded **Ph.D. in Physical Chemistry**
 Principal Subjects/Occupational Skills Covered Thesis Title: "Modeling of the Influence of Molecule Rotation on the Kinetic of Thermal Unimolecular Reactions" (Magna cum laude).
 Name and Type of Organisation Providing Education and Training University of Karlsruhe (TH), Karlsruhe, Germany
 Level in National or International Classification ISCED 6
 Date 1990
 Title of Qualification Awarded **M.Sc. in Biology and Chemistry**
 Principal Subjects/Occupational Skills Covered **Thesis Title:** "Physical-Chemical Investigation of Complex Compounds of Zn(II) and Cu(II) with the Pyridine Carbon Acids" (Graduated with honor; GPA: 4.0).
 Name and Type of Organisation Providing Education and Training Tbilisi State Pedagogical University, Georgia
 Level in National or International Classification ISCED 5

Personal Skills and Competences

Mother Tongue(s) **Georgian**
 Other Language(s) **German, English, Russian**
 European level (*)

	Understanding		Speaking		Writing
	Listening	Reading	Spoken interaction	Spoken production	Writing
English	C2 Very good	Very good	Very good	Very good	Good
German	C2 Very good	Very good	Very good	Very good	Very good
Russian	C2 Very good	Very good	Very good	Very good	Good

Social Skills and Competences Personal commitments as well as the ability to motivate others, team spirit and the ability to listen, to understand, and to integrate others' opinions; strong communication skills; interest in other countries and profound respect for their cultures

Organisational Skills and Competences Experience in project management, leadership skills, organizational skills

Computer Skills and Competences	<p>Programming Languages: FORTRAN 77/90/95, Shell Scripting, Perl, Mathematica</p> <p>Operating Systems: UNIX/LINUX, Windows, Mac OS X</p> <p>Scientific Software: GAUSSIAN, MOLPRO, NWChem, SPARTAN, TURBOMOLE, GAMESS, MOPAC VENUS, POLYRATE, VARIFLEX, MM32000, Venus-NWchem</p> <p>Other Skills: Cross platform Qt C++ GUI toolkit; portable C++/FORTRAN mixed language toolkit; MATHEMATICA, ORIGIN, KaleidaGraph, MOLDEN, VMD, GNUPLOT, MS Office</p> <p>Microsoft Office (Word, Excel, PowerPoint, Access, Macros), Adobe Acrobat, LaTeX, image editing (Adobe Photoshop, Designer)</p>
Other Skills and Competences	Quick learner; able to adapt to different situations/problems; goal-oriented; hard-worker
Driving License	US and Georgian driving license (Category B)
Honors and Fellowships	<p>DAAD Fellow, September 1998 – July 1999</p> <p>36th International Seminar for Research and Teaching in Chemical Engineering and Physical Chemistry, University of Karlsruhe (TH), Germany</p> <p>University Fellow 1988-1990</p> <p>Tbilisi State Pedagogical University, Georgia</p>
Trainings	<p>Alumni relations, Tbilisi State University, Tbilisi, Georgia (2010)</p> <p>Learner-centered education, Tbilisi State University, Tbilisi, Georgia (2009)</p> <p>Molpro Workshop, Stuttgart, Germany (2003)</p> <p>DECHEMA-Seminars, Frankfurt, Germany (1998-1999)</p> <p>Forschungszentrum Karlsruhe, Karlsruhe, Germany (1998)</p>

PUBLICATION LIST

Khatuna Kakhiani

- “Cyclohexane Isomerization. Unimolecular Dynamics of the Twist Boat Intermediate”, **Khatuna Kakhiani**, Upakarasamy Lourderaj, Wenfang Hu, David Birney, and William L. Hase, *J. Phys. Chem. A*, 113(6), 4570-4580, (2009).
- “A Program to Generate a Basis Set Adaptive Radial Quadrature Grid for Density Functional Theory”, **K. Kakhiani**, K. Tsereteli, and P. Tsereteli, *Computer Physics Communications*, 180, 256–268, (2009).
- “Shock Wave Study on the Thermal Unimolecular Decomposition of Allyl Radicals”, R. X. Fernandes, B. R. Giri, H. Hippler, **C. Kachiani**, and F. Striebel, *J. Phys. Chem. A.*, 109(6), 1063-1070, (2005).
- Ph.D Thesis: „Modellierung des Einflusses der Molekülrotation auf die Kinetik thermischer unimolekularer Reaktionen“, **Chatuna Kachiani**, Cuvillier Verlag Göttingen, 2004, ISBN 3-86537-156-6 (in German).
- “Rotational Effects in Multi-Channel Unimolecular Reactions”, H. Hippler, C. Kachiani, and M. Olzmann, *European Combustion Meeting “ECM2003”*, October 25-28, 2003, Orléans, France.
- “Collisional Energy Transfer in CH₃ Radical Decomposition-Experiment Versus Theory”, E. Goos, H. Hippler, **C. Kachiani**, and H. Svedung, *Phys. Chem. Chem. Phys.*, 4(18), 4372-4378, (2002).
- “Incubation Times, Fall-Off and Branching Ratios in the Thermal Decomposition of Toluene: Experiments and Theory”, R. A. Eng, A. Gebert, E. Goos, H. Hippler, and **C. Kachiani**, *Phys. Chem. Chem. Phys.*, 4(16), 3989-3996, (2002).
- “Branching Ratios and Incubation Times in the Thermal Decomposition of Methyl Radicals: Experiments and Theory”, R. A. Eng, A. Gebert, E. Goos, H. Hippler, and **C. Kachiani**, *Phys. Chem. Chem. Phys.*, 3(12), 2258-2267, (2001).
- G. V. Tsintsadze, E. S. Topuria, M. G. Tsintsadze, **Kh. Kakhiani**, R. Sh. Kurtanidze, and K. N. Tsereteli, *Izvestia Akademii Nauk Gruzii, Seria Khimicheskaya*, 26(3-4), 44-50, (2000) in Russian.

ORAL PRESENTATIONS

- Kakha Tsereteli and Khatuna Kakhiani, “Modeling of Electron Transfer in Dye-Sensitized Solar Cells”, DAAD Alumni Workshop “Renewable Energy”, Thessaloniki, Greece, May 16th – 22nd, (2010).
- Kakha Tsereteli and **Khatuna Kakhiani**, “Nonadiabatic Molecular Dynamics Modeling of Electron Transfer in Dye-Sensitized Solar Cells”. *Material Science Days*, Tbilisi State University, Tbilisi, Georgia, 8-9 July (2009).
- **Kakhiani, Khatuna**; Birney, David M.; Lourderaj, Upakarasamy; Hase, William L. *Dynamics of Cyclohexane Isomerization. 63rd Southwest Regional Meeting of the American Chemical Society*, Lubbock, TX, USA, November 4-7 (2007).
- **K. Kakhiani**, Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, USA (9.2.2007).

- **C. Kachiani**, R. A. Eng, A. Gebert and H. Hippler, *Bunsentagung*, 2001, Stuttgart, Germany.

POSTER PRESENTATIONS

- **K. Kakhiani**, *21st International Symposium on Gas Kinetics*, 2010, Katholieke Universiteit Leuven, Leuven, Belgium.
- **K. Kakhiani**, L. B. Harding, A. F. Wagner, *6th International Conference on Chemical Kinetics*, 2005, NIST, Gaithersburg, MD, USA.
- H. Hippler, **C. Kachiani**, and M. Olzmann, *European Combustion Meeting "ECM2003"*, October 25-28, 2003, Orléans, France.
- R. Fernandes, H. Hippler, **C. Kachiani**, M. Olzmann, and F. Striebel, *European Combustion Meeting "ECM2003"*, October 25-28, 2003, Orléans, France.
- H. Hippler and **C. Kachiani**, *17th International Symposium on Gas Kinetics*, 2002, Universität Essen, Germany.
- E. Goos, H. Hippler, C. Kachiani, and H. Svedung, *17th International Symposium on Gas Kinetics*, 2002, Universität Essen, Germany.
- R. A. Eng, A. Gebert, H. Hippler, **C. Kachiani**, *International Discussion Meeting: Competitive Processes in Vibrationally Highly Excited Molecules*, October 4-5, 2000, Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany.