SOPHYA GARASHCHUK

Professor
Department of Chemistry and Biochemistry
University of South Carolina 803-777-8900
Columbia, SC 29208 garashch@mailbox.sc.edu
https://sc.edu/study/colleges_schools/chemistry_and_biochemistry/our_people/directory/garashchuk_sophya.php

PROFESSIONAL PREPARATION

Institution	*Area*	*Degree/Year*	
Moscow Institute of Physics and Technology			
Russia	Physics	MS Magna Cum Laude	1992
University of Notre Dame, IN	Physics	Ph. D.	1998
University of Chicago, IL	Chemistry	postdoc	1999-2001

APPOINTMENTS

2019-present	Professor of Chemistry	U of South Carolina
2013-2018	Associate Professor of Chemistry	U of South Carolina
2008-2013	Assistant Professor of Chemistry	U of South Carolina
2002-2004, 2007	Assistant Research Professor/Chemistry	U of South Carolina
2005-2006	Research Associate/Chemistry	Northwestern U

ACCOLADES

SC Chemist of the Year (SC ACS), 2026
USC Carreer Influencer, 2025

Visiting Research Fellowship, Maks Planck Institute for the Physics of Complex Systems, Dersden, Germany 2023

USC Rising Star, 2012

Doctoral New Investigator ACS Petroleum Research Fund, 2011

National Science Foundation: Career, 2011

IBM-Lowdin Fellowship, Sanibel symposium 2004

RESEARCH INTERESTS

Theoretical and computational chemistry: theory of quantum, classical and semiclassical reaction dynamics; scattering theory; simulation of quantum effects due to nuclear motion in large systems (reactions coupled to molecular environment and in condensed phase); role of the nuclear quantum effects on properties of materials

SELECTED PUBLICATIONS

out of 93 peer-reviewed papers listed at **https://orcid.org/my-orcid?orcid=0000-0003-2452-7379**

1. *Factorised electron-nuclear dynamics with effective complex potential: on-the-fly implementation for H_2^+ in a laser field.* Stetzler, J., Garashchuk, S., & Rassolov, V. Molecular Physics (**2026**) https://doi.org/10.1080/00268976.2025.2611404
2. *Variational Dynamics of Multicomponent Wave Functions Represented in a Basis Driven by a Time-Dependent Gaussian Wavepacket.* Sophya Garashchuk, Julian Stetzler, Chanikya D. Jayawardana, Michael Anim Safo, and Vitaly A. Rassolov. Journal of Chemical Theory and Computation (**2025**) 21 (15), 7249-7266. DOI: 10.1021/acs.jctc.5c00640
3. *Theoretical Examination of the Hydroxide Transport in Cobaltocenium-Containing Polyelectrolytes.* Sachith Wickramasinghe, Alexandria Hoehn, Shehani T. Wetthasinghe, Huina Lin, Qi Wang, Jacek Jakowski, Vitaly Rassolov, Chuanbing Tang, and Sophya Garashchuk. The Journal of Physical Chemistry B (**2023**) 127 (47), 10129-10141. DOI: 10.1021/acs.jpcb.3c04118
4. *Stability Analysis of Substituted Cobaltocenium [Bis(cyclopentadienyl)cobalt(III)] Employing Chemistry-Informed Neural Networks*. Chunyan Li, Shehani T. Wetthasinghe, Huina Lin, Tianyu Zhu, Chuanbing Tang, Vitaly Rassolov, Qi Wang, and Sophya Garashchuk. Journal of Chemical Theory and Computation (**2022)** 18 (5), 3099-3110. DOI: 10.1021/acs.jctc.1c01201
5. *"Broken-Hearted" Carbon Bowl via Electron Shuttle Reaction: Energetics and Electron Coupling.* Leith, Gabrielle A; Rice, Allison M; Yarbrough, Brandon J; Kittikhunnatham, Preecha; Mathur, Abhijai; Morris, Nicholas A; Francis, Megan J; Berseneva, Anna A; Dhull, Poonam; Adams, Richard D; Bobo, M Victoria; Vannucci, Aaron K; Smith, Mark D; Garashchuk, Sophya; Shustova, Natalia. Chemical Science (**2021**).
6. *Molecular dynamics with nuclear quantum effects: Approximations to the quantum force.* S. Garashchuk, V. A. Rassolov. Annual Reports on Computational Chemistry 16 (**2020**), 41 pages, Elsevier.
7. *Relevance of the Nuclear Quantum Effects on the Proton/Deuteron Transmission through Hexagonal Boron Nitride and Graphene Monolayers.* N. T. Ekanayake, J. Huang, J. Jakowski, B. G. Sumpter, S. Garashchuk. J. Chem. Phys. C. **121**:24335–24344 (**2017**) http://dx.doi.org/10.1021/acs.jpcc.7b08152
8. *Deuteration as a Means to Tune Crystallinity of Conducting Polymers.* J. Jakowski, J. Huang, S. Garashchuk, Y. Luo, K. Hong, J. Keum, B. G. Sumpter. J. Phys. Chem. Lett. 8, 4333-4340 (**2017**), http://dx.doi.org/10.1021/acs.jpclett.7b01803
9. *Understanding How Isotopes Affect Charge Transfer in P3HT/PCBM: A Quantum Trajectory-Electronic Structure Study with Nonlinear Quantum Corrections.* L. Wang, J. Jakowski, S. Garashchuk, B. G. Sumpter. J. Chem. Theory Comp. 12, 4487-4500 (**2016**), http://dx.doi.org/10.1021/acs.jctc.6b00126
10. *Quantum Trajectory-Electronic Structure Approach for Exploring Nuclear Effects in the Dynamics of Nanomaterials.* S. Garashchuk, J. Jakowski, L. Wang and B. G. Sumpter. J. Chem. Theory and Comp. 9, 5221--5235 (**2013**) http://pubs.acs.org/doi/abs/10.1021/ct4006147

COLLABORATORS & OTHER AFFILIATIONS

1. Collaborators (last five years). ORNL: J. Jakowski, B. G. Sumpter, J. Hong; UofSC: V. A.

Rassolov, N. Shustova, L. Shimizu, C. Tang, A. Vannucci, M. Stefik, Q. Wang
2. Mentors: D. J. Tannor (The Weizmann Institute of Science, Ph.D. mentor), J. C. Light (U of Chicago, postdoctoral mentor)

RESEARCH SUPERVISION

Post-doctoral supervision

Tijo Vazhappilly	01/2009 – 01/2011
Mikhail Volkov	09/2011 – 06/2012
Susanta Ghanta	01/2012 – 04/2012
Lei Wang	08/01/12 – 08/01/15
David Dell'Angelo	08/01/12 – 5/31/14
Matt Dutra	2018 – 2022
Shehani Wetthasinghe	2024 – 2025
Giacomo Botti	2025 – present

Graduate supervision

James Mazucca	Ph.D. 2014
Bing Gu	Ph.D. 2016
Sachith Wickramasinghe	Ph.D. 2023
Niranji Ekanayake	M.Sc. 2018
Austin Hill	M.Sc. 2024
Julian Stetzler	01/2022 – current
Michael Safo	01/2023 – current

Undergraduate and Pre-College supervision ~ 25 students since 2010

TEACHING

1. CHEM 142 Honors General Chemistry II
2. CHEM 112 General Chemistry II
3. CHEM 542 Physical Chemistry II – Quantum Mechanics and Spectroscopy
4. CHEM 743 Quantum Chemistry (graduate)
5. CHEM 749/643Computational Chemistry (graduate/undergraduate)

SYNERGISTIC ACTIVITIES AND SELECTED SERVICE

1. Facilitating access to Computational Chemistry resources at USC
2. Computational chemistry education and outreach: development of the computational chemistry laboratories for chemistry majors (general, organic labs, and physical chemistry recitations) and of the undergraduate/graduate course 'Computational Chemistry'. A faculty for AI4Science summer camp for high-school student https://cse.sc.edu/news/successful-inauguration-2024-south-carolina-ai4science-summer-camp
3. Mentor, reviewer and judge for the Magellan Scholar program funding undergraduate research
4. Reviewer for 18 physics and chemistry journals and several funding agencies
5. Virtual International Seminar for Theory Advancement (VISTA) – executive committee

member (2023-current) https://quantum-dynamics-hub.github.io/VISTA/