

Curriculum Vitae

Sophya Garashchuk

Professor
Department of Chemistry and Biochemistry
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Professional preparation:

Moscow Institute of Physics and Technology, Moscow, Russia
MS Magna Cum Laude, 1992
University of Notre Dame, IN, Ph. D. Physics, 1998
University of Chicago, The James Franck Institute, Postdoctoral Fellow, 1999-2001

Research and Professional Experience:

Professor, Dept of Chemistry and Biochemistry, University of South Carolina, since 2019
Associate Professor, Dept of Chemistry and Biochemistry, University of South Carolina 2013-2018
Assistant Professor, Dept of Chemistry and Biochemistry, University of South Carolina 2008-2012
Assistant Research Professor, University of South Carolina 2002-2004, 2007-2008
Research Associate, Northwestern University, 2005-2006

Significant Awards and Honors:

Fellowship at Max Planck Institute for Physics of Complex Systems, Dresden, Germany, Mar-July 2023
Visiting Scientist at California Institute of Technology, Pasadena, California, Nov 2016
Visiting Scientist at University of New South Wales, Canberra, Australia, May-June 2016
USC Rising Star, 2012; Doctoral New Investigator ACS Petroleum Research Fund, 2011; National Science Foundation: Career, 2011; IBM-Lowdin Fellowship, Sanibel symposium 2004

Teaching:

General chemistry CHEM142M, CHEM112
Physical chemistry CHEM542
Quantum chemistry CHEM743/649

Selected Professional Activities (last 5 years):

1. Development and deployment of computational chemistry laboratories for undergraduates (general and organic chemistry) and Computational Chemistry course, user training in chemistry software on HPC
2. Reviewer for 18 physics and chemistry journals and for the NSF, DOE, PRF-ACS, UofSC funding agencies; panel reviewer; tenure and promotion reviewer
3. Co-chair, Southeast Theoretical Chemistry Conference, USC, Columbia, SC, May 2010 and May 2023
Organizer of Computational and Physical Chemistry sessions at SERMACS, Columbia, SC, Oct 2016
4. Member, University Senate Information Technology committee (2018-2020) and Faculty focus group (2021), USC HPC faculty advisory (2019-current)
5. ACS and AAAS member

Number of Articles Published in Peer Reviewed Journals: 80+ ORCID [0000-0003-2452-7379](https://orcid.org/0000-0003-2452-7379)

Selected publications:

1. *Chapter 3 - From classical to quantum dynamics of atomic and ionic species interacting with graphene and its analogue.* Sophia Garashchuk, Jingsong Huang, Bobby G. Sumpter, Jacek Jakowski. *Theoretical and Computational Chemistry*, Elsevier, Volume **21** (2022), 61-86.
<https://doi.org/10.1016/B978-0-12-819514-7.00001-4>.
2. *Approximate quantum trajectory dynamics for reactive processes in condensed phase.* S. Garashchuk, J. Jakowski, and V. A. Rassolov. *Molecular Simulation*, **41**(2015),1–21.
<http://www.tandfonline.com/doi/abs/10.1080/08927022.2014.907493>
3. *Factorized Electron–Nuclear Dynamics with an Effective Complex Potential.* Sophia Garashchuk, Julian Stetzler, Vitaly Rassolov. *J. Chem. Theory and Comput.* 2023, 19, 5, 1393–1408, DOI: [10.1021/acs.jctc.2c01019](https://doi.org/10.1021/acs.jctc.2c01019)
4. *A Metal-Organic Framework (MOF)-Based Multifunctional Cargo Vehicle for Reactive-Gas Delivery and Catalysis* P. Kittikhunnatham, G. A. Leith, A. Mathur, J. K. Naglic, C. R. Martin, K. C. Park, K. McCullough, H. D. A. C. Jayaweera, R. E. Corkill, J. Lauterbach, S. G. Karakalos, M. D. Smith, S. Garashchuk, D. A. Chen, N. B. Shustova, *Angew. Chem. Int. Ed.* **2022**, *61*, e202113909; *Angew. Chem.* **2022**, *134*, e202113909.
5. *Stability Analysis of Substituted Cobaltocenium [Bis(cyclopentadienyl)cobalt(III)] Employing Chemistry-Informed Neural Networks.* Chunyan Li, Shehane T. Wetthasinghe, Huina Lin, Tianyu Zhu, Chuanbing Tang, Vitaly Rassolov, Qi Wang, and Sophia Garashchuk
Journal of Chemical Theory and Computation 2022 18 (5), 3099-3110 DOI: 10.1021/acs.jctc.1c01201

Key Collaborators:

J. Jakowski (ORNL); V. A. Rassolov (USC), N. Shustova (UofSC), L. Shimizu (USC), C. Tang (USC), Qi Qiang (USC), D. Chen (USC), T. Makris (NCU)

Graduate and Postdoctoral Advisors:

David Tannor (Weizmann Institute); John Light (U Chicago)

Graduate Students: James Mazzuca (Alma College), Bing Gu (Westlake U), Niranji Ekanayake, Sachith Wickramasinghe (USC), Austin Hill (USC), Julian Stetzler (USC)

Postdoctoral Scholars: D. Dell'Angelo, 2012-2013; S. Ghanta, 01/2012-03/2012; W. Lei, 2013-2015; T. Vazhappilly, 2009-2011; M. Volkov, 2011-06/2012; M. Dutra 2018-2022

Mentorship of recent USC undergraduate researchers:

Shannon McElhenney (UC-Irvine), Sasha Sawyer (U Washington), Carson Tang (U Georgia), Alexandria Hoehn (U Chicago), Cathryn Murphy (Northwestern U)