Curriculum Vitae

Sophya Garashchuk

Professor

Department of Chemistry and Biochemistry

University of South Carolina

Columbia, SC 29208

803-777-8900

garashchuk@sc.edu

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; Physical chemistry CHEM542; Quantum chemistry CHEM743; Computational chemistry CHEM643

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 ~20 physics and chemistry journals and for the NSF, DOE, PRF-ACS, USC 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. Committee Member for the Petroleum Research Fund of the American Chemical Society (2024-current)

Number of Articles Published in Peer Reviewed Journals: 90+ ORCID 0000-0003-2452-7379

Selected publications:

1. 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, Vitaly A. Rassolov. J. Chem. Theory and Comput. 2025, 15, 7249-7266. https://doi.org/10.1021/acs.jctc.5c00640

2. Factorized Electron–Nuclear Dynamics with an Effective Complex Potential. Sophya Garashchuk, Julian Stetzler, Vitaly Rassolov. J. Chem. Theory and Comput. 2023, 19, 5, 1393–1408, DOI: 10.1021/acs.jctc.2c01019

3. 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.

4. Chapter 3 - From classical to quantum dynamics of atomic and ionic species interacting with graphene and its analogue. Sophya 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.

5. 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, J. Chem. Theory and Comp. 2022 18 (5), 3099-3110 DOI: 10.1021/acs.jctc.1c01201

Key Collaborators:

J. Jakowski (ORNL); V. A. Rassolov (USC), N. Shustova (USC), L. Shimizu (USC), C. Tang (USC), Qi Qang (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 (UT Austin), Austin Hill, Julian Stetzler (USC), Michael Safo (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; S. Wetthasinghe (2024-), G. Botti (2025-)

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)