Philip Shushkov

Department of Chemistry • Indiana University

PROFESSIONAL APPOINTMENT

Indiana University Assistant Professor of Chemistry Tufts University Charles W. Fotis Assistant Professor of Chemistry	Bloomington, IN 2022 – present Medford, MA 2020 – 2022
EDUCATION	
Yale University Ph.D. Chemistry Sofia University M.S. Sofia University B.S.	New Haven, CT 2008 – 2013 Sofia, Bulgaria 2006 – 2008 Sofia, Bulgaria 2002 – 2006
POSTDOCTORAL TRAINING	
California Institute of Technology DFG postdoctoral fellow Mulliken Center for Theoretical Chemistry Alexander von Humboldt Fellow	Pasadena, CA 2017 – 2020 Bonn, Germany 2013 – 2016
FELLOWSHIPS AND AWARDS	
NSF CAREER Award	2025 - 2030
DOE Early Career Award	2024 – 2029
German Research Foundation (DFG) Fellowship	2017 – 2019
Alexander von Humboldt Fellowship	2014 – 2016
Richard Wolfgang Prize for best doctoral thesis in Chemistry Yale University	2013
Dean's Distinction Award for outstanding achievements Sofia University	2008
Valedictorian of Bachelor Class Award Sofia University	2006

PUBLICATIONS

Ph. Shushkov, *A Novel Non-adiabatic Spin Relaxation Mechanism in Molecular Qubits*, J. Chem. Phys. **160**, 164105 (2024).

A. Demling, S. B. King, **Ph. Shushkov**, and J. Stähler, *O*₂ *Reduction at a DMSO/Cu*(*111*) *Model Battery Interface*, J. Phys. Chem. C **127**, 2894 (2023).

X. Tao, **Ph. Shushkov**, and T. F. Miller III, *Microcanonical Rates from Ring-Polymer Molecular Dynamics: Direct-Shooting, Stationary-Phase, and Maximum-Entropy Approaches*, J. Chem. Phys. **152**, 124117 (2020). J. Chem. Phys. *Editor's Choice*

Ph. Shushkov[#] and T. F. Miller III, *Real-Time Density-Matrix Coupled-Cluster Approach for Closed and Open Systems at Finite Temperature*, J. Chem. Phys. **151**, 134107 (2019). J. Chem. Phys. *Featured Article* and *Editor's Choice* [#]indicates corresponding author

Y. Yao^{*}, **Ph. Shushkov**^{*}, T. F. Miller III, and K. P. Giapis, *Direct Dioxigen Evolution in Collisions of Carbon Dioxide with Surfaces*, Nature Communications **10**, 2294 (2019). *indicates co-first authorship

X. Tao, **Ph. Shushkov**, and T. F. Miller III, *A Simple Flux-Side Formulation of State-Resolved Thermal Reaction Rates for Ring-Polymer Surface Hopping*, J. Phys. Chem. A **123**, 3013 (2019).

X. Tao, **Ph. Shushkov**, and T. F. Miller III, *Path-Integral Isomorphic Hamiltonian for Including Nuclear Quantum Effects in Non-adiabatic Dynamics*, J. Chem. Phys. **148**, 102327 (2018).

S. Grimme, C. Bannwarth, and **Ph. Shushkov**, *A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements (Z = 1–86),* J. Chem. Theory Comput. **13**, 1989 (2017).

C. Schweez^{*}, **Ph. Shushkov**^{*}, S. Grimme, and S. Höger, *Synthesis and Dynamics of Nanosize Phenylene-Ethynylene-Butadiynylene Rotaxanes and the Role of Shape Persistence*, Angew. Chem. Int. Ed. **55**, 3328 (2016). *indicates co-first authorship

Ph. Shushkov, On the Connection of Semiclassical Instanton Theory with Marcus Theory for Electron Transfer in Solution, J. Chem. Phys. **138**, 224102 (2013). J. Chem. Phys. Editor's Choice

F. Evangelista, **Ph. Shushkov**, and J. C. Tully, *Orthogonality Constrained Density Functional Theory for Electronic Excited States*, J. Phys. Chem. A **117**, 7378 (2013). featured in *Developments in Theoretical Chemistry*

Ph. Shushkov, R. Li, and J. C. Tully, *Ring Polymer Molecular Dynamics with Surface Hopping*, J. Chem. Phys. **137**, 22A549 (2012).

M. Velinova, Y. Tsoneva, **Ph. Shushkov**, A. Ivanova, and A. Tadjer, *Systematic Derivation and Testing of AMBER Force Field Parameters for Fatty Ethers from Quantum Mechanical Calculations*, Prog. Theor. Chem. Phys. **22**, 461 (2012).

R. Steele, J. Zwickl, **Ph. Shushkov**, and J. C. Tully, *Mixed Time Slicing in Path Integral Simulations*, J. Chem. Phys. **134**, 074112 (2011).

Ph. Shushkov, S. Tzvetanov, M. Velinova, A. Ivanova, and A. Tadjer, *Structural Aspects of Lipid Monolayers: Computer Simulation Analyses*, Langmuir **26**, 8081 (2010).

S. Tzvetanov, **Ph. Shushkov**, M. Velinova, A. Ivanova, and A. Tadjer, *Molecular Dynamics Study of the Electric and Dielectric Properties of Model DPPC and Dicaprin Insoluble Monolayers: Size Effect*, Langmuir **26**, 8093 (2010).

A. Ivanova, **Ph. Shushkov**, and N. Rosch, *Systematic Study of the Influence of Base-step Parameters on the Electronic Coupling between Base-pair Dimers: Comparison of A-DNA and B-DNA Forms*, J. Phys. Chem. A **112**, 7106 (2008).

Ph. Shushkov, S. Tzvetanov, A. Ivanova, and A. Tadjer, *Dielectric Properties Tangential to the Interface in Model Insoluble Monolayers: Theoretical Assessment*, Langmuir **24**, 4615 (2008).

SELECTED PRESENTATIONS

2024	<i>"Spin dynamics of molecular qubits"</i>MAGNA, February 2025
2024	 <i>"Non-adiabatic spin-relaxation mechanism in molecular qubits"</i> TSRC, Molecular Qubits, June 2024
2023	 <i>"Spin-relaxation dynamics of molecular spin qubits"</i> ACS San Francisco, August 2023 Sanibel, Quantum Chemistry Conference, February 2023
2022	 <i>"Quantum dynamics of molecular spin systems"</i> TSRC "Condensed Phase Dynamics", July 2022 ACS Chicago, Quantum Chemistry Symposium, August 2022
2022	 <i>"Chemical dynamics from surfaces to quantum information science: new methods for quantum dynamics at finite temperature"</i> Indiana University, April 2022 University of Zurich, March 2022
2021	 "Coupled cluster dynamics at finite temperature: Quantum statistics and Ehrenfest theorem" TSRC "New Frontiers in Electron Correlation", virtual, June 2021
2020	 "Coupled cluster methods for the dynamics of closed and open systems at finite temperature" TSRC "Condensed Phase Dynamics", virtual, July LUEST TSRC, virtual, June 2020

TEACHING EXPERIENCE

Indiana University	Bloomington, IN
Instructor, Quantum Mechanics	2024
Instructor, Physical Chemistry of Bulk Matter	
Instructor, Physical Chemistry of Bulk Matter	2023
Instructor, Quantum Mechanics	
Tufts University	Medford, MA
Instructor, Theoretical Chemistry Methods	2022
Instructor, Quantum Mechanics	2021
Instructor, Physical Chemistry I	2020