CURRICULUM VITAE

Spiridoula Matsika, Ph.D
Department of Chemistry, Temple University
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EDUCATION

Ph.D. in Chemical Physics; The Ohio State University, Columbus, OH, USA; 2000

Thesis Title:	Relativistic Effects in the Spectroscopy of Actinyl Compounds and Weakly Bound Complexes
Adviser:	Professor Russell M. Pitzer

B. Sc. in Chemistry; The National and Kapodistrian University of Athens, Athens, Greece; 1994

APPOINTMENTS

2014 - present	Professor, Temple University
2009 -2014	Associate Professor, Temple University
2003 -2009	Assistant Professor, Temple University
2000-2003	Postdoctoral Fellow, Johns Hopkins University

AWARDS

- ACS Philadelphia Section Award, 2025
- The Dean's Distinguished Award for Excellence in Research, Temple University, 2016
- Co-chair Gordon Research Conference on Molecular Interactions and Dynamics, 2016
- Fellow of the American Physical Society, 2014
- Alexander von Humboldt Fellow, 2013
- Löwdin Lecturer, 2012
- NSF CAREER Award, 2005
- Presidential Fellowship, The Ohio State University, 1999-2000

MEMBERSHIPS IN PROFESSIONAL ORGANIZATIONS

- American Physical Society
- American Chemical Society

TEACHING ACTIVITIES:

S 04	Chem 636: Molecular Spectroscopy
F 04, 05, 06, 08, 09, 16, 19, 21, 23, 25	Chem 5301: Quantum Chemistry
S 05, 07, 09, 12, 17, F 07, 14	Chem 3302: Physical Chemistry II
S 06	Chem 738: Special Topics in Phys. Chem: Computational Chemistry
S 08, 13, 15, 24, 25, F 17, 18, 20, 22	Chem 8302: Computational Chemistry
S 10, 11, 14, F 12	Chem 5305: Chemical Kinetics
F 11	Chem 8300: Special Topics in Phys. Chem: Adv.Quantum Chemistry
S 18, 19, 21, 22	Chem 3405: Physical Chemistry of Biomolecules
S 20	Chem 4301: Advanced Physical Chemistry

SERVICE ACTIVITIES:

Departmental:

2003-2005, 2007-2008	Presidential Faculty Search Committee
Summer 2004-2007	Graduate Recruiting Committee
Spring 2007-2016	Graduate Admissions Committee
Fall 2007-2021	Undergraduate Curriculum Analysis and Development Committee
Fall 2014-2019	Chair, Undergraduate Curriculum Analysis and Development Committee
Fall 2009-2021	Undergraduate Faculty Advisor
Spring 2021-present	Graduate Committee
Spring 2022-present	DEI Committee
Fall 2023-2024	Awards Committee
Fall 2025	Vice Chair, Department of Chemistry

Collegial:

Fall 2010-2011	Student Grievance Committee
Fall 2009-2014	CST Undergraduate Committee
Fall 2010-2014, 2020-2022	CST Merit Committee
Fall 2013-2014	Chair, CST Merit Committee
Fall 2014	Mathematics Faculty Search Committee
Fall 2015 - 2020	CST Tenure and Promotion Committee
Fall 2019 - 2020	Chair, CST Tenure and Promotion Committee
Fall 2019	Physics Faculty Search Committee
Fall 2023	Research Award Committee

Professional:

Associate Editor	Physical Chemistry Chemical Physics, 2023- present
Director:	"Maximizing Access to Research Careers" at Temple University, funded by NIH (2020- present)
Reviewer:	(Journals) JACS, JPC, IC, PRL, CPLett., IJMS, Chem. Phys., JCTC, JPOC, JCP, Photochem. Photobiology, J. Photoch. Photob.A, Tetrahedron, PCCP, JOC, ChemPhysChem, ARPC, Chem. Rev., Nature, Nature Chem, PNAS, Angewandte, Frontiers in Bioengin., WIREs, Biophys. Chem., Science, Adv. Quantum Chem. (Agencies: reviewed individual proposals and/or served on panels) NSF, PRF, DOE, AFOSR, ERC ISF, NIH: Training and Workforce Development Study Section - C (2022-2024)
Organizer:	Symposium at National ACS meeting, Boston 2007 (co-organized with Todd Martinez) Symposium for MARM 2007 Mini-Symposium in honor of Russell Pitzer, 63rd OSU International Symposium on Molecular Spectroscopy (co-organized with Anne McCoy), 2008 Workshop, "The Science of Performance", for high school students from the Carver High School of Engineering and Science, 2006 Mini-Symposium on "Conical Intersections", 64th OSU International Symposium on Molecular Spectroscopy (co-organized with Scott Reid), 2009 Member of the Jahn-Teller Symposium steering committee 2009-present American Physical Society Focus session on Nonadiabatic Dynamics, San Antonio, March 2015 Gordon Research Conference on Molecular Interactions and Dynamics (2016) Telluride workshop on "Molecular Spectroscopy and Dynamics", Telluride, 2024-present Focus Session "Nonadiabatic Chemical Dynamics – Theory and Experiments." at the APS Global Summit, March 2026 (co-organized with Krupa Ramasesha)
Member:	Editorial Advisory Board of the Journal of Physical Chemistry, 2014-2016, 2021-2023 Committee of Sciences and the Arts (CSA) of the Franklin Institute, 2014-present Editorial Committee of the Annual Review of Physical Chemistry, 2016- 2022 American Physical Society, DCP nominating committee, 2017-2019 Editorial Advisory Board of Physical Chemistry Chemical Physics, 2019-present Editorial Advisory Board of the Journal of Chemical Physics, 2020-2022 DAMOP Program Committee 2021-2024 Faculty promotion committee, University of Athens, GR, 2020 -2022 Faculty promotion committee, University of Patras, GR, 2025 Faculty promotion committee, University of Ioannina, GR, 2025
Guest editor	Journal of Physical Chemistry A, Russell M. Pitzer Festschrift, 2009 Journal of Physical Chemistry A, David R. Yarkony Festschrift, 2014 Chemical Reviews thematic issue on "Theoretical Modeling of Excited-State Processes", 2017 Chemical Physics, W. Domcke Festschrift, 2018 Phys.Chem.Chem.Phys special issue on "Developments in Ultrafast Spectroscopy", 2022 Book published by Springer "Nucleic Acid Photophysics and Photochemistry", 2024 Phys.Chem.Chem.Phys special issue in memory of David R. Yarkony 2025
Outreach:	CATALYST leader: workshop for middle school girls, Swarthmore College, March 2012, 2015 Panel EMB, Women in STEM, Engineering in Medicine and Biology IEEE AUTh, May 2024 Advocate about science funding to senators in PA, July 2025

PUBLICATIONS
(156 total (h index=36 (Web of Science), h index=46 (Google Scholar)))

1. "Partial Widths of Shape Resonances in Pyridine and Uracil Using the Orbital Stabilization Method", Maneesh Pyla, Spiridoula Matsika, *J. Chem. Phys.*, submitted (2025)
2. "Statistical vs Direct Dissociation of Molecular Dications" Vaibhav Singh, Kovi Bodek, Gönenç Moğol, Chuan Cheng, Carlos A Trallero-Herrero, Thomas Weinacht, and Spiridoula Matsika *Phys. Chem. Chem. Phys.*, accepted (2025)
3. "How excitation wavelength affects excited state dynamics in o-nitrophenol: A theoretical perspective", Dakshitha Abeygunewardane, Thomas Weinacht, Spiridoula Matsika, *J. Chem. Phys.*, **163**, 024314 (2025) https://doi.org/10.1063/5.0274633
4. "COLUMBUS — an Efficient and General Program Package for Ground and Excited State Computations Including Spin-Orbit Couplings and Dynamics ", Felix Plasser, Hans Lischka, Ron Shepard, Péter G. Szalay, Russel M. Pitzer, Rodolpho L. R. Alves, Adelia A. J. A. Aquino, Jochen Autschbach, Mario Barbatti, Jhonatas R. Carvalho, Julio C. V. Chagas, Leticia González, Andreas Hansen, Bhumika Jayee, Miklos Kertesz, Francisco B. C. Machado, Spiridoula Matsika, Silmar A. do Monte, Saikat Mukherjee, Dana Nachtigallová, Reed Nieman, Vytor P. Oliveira, Markus Oppelt, Carol A. Parish, Jiri Pittner, Luan G. F. dos Santos, Armin Scrinzi, Mahesh K. Sit, Rene F. K. Spada, Mushir Thodika, Álvaro Vázquez-Mayagoitia, Daniel C. A. Valente, Elizete Ventura, Julia Westermayr, Aleksandr Zaichenko, Zhiyong Zhang, *J. Phys. Chem. A*, **129**, 6482–6517 (2025) https://doi.org/10.1021/acs.jpca.5c02047
5. "Impact of Solvation on the Two Particle One Hole Resonance in Uracil " Divya Tripathi, Maneesh Pyla, Achintya Kumar Dutta, Spiridoula Matsika, *Phys. Chem. Chem. Phys.*, **27**, 3588-3601, (2025) https://doi.org/10.1039/D4CP04333B
6. "Ultrafast structural dynamics of UV photoexcited cis,cis-1,3- cyclooctadiene observed with femtosecond electron diffraction", Sri Bhavya Muvva1, Yusong Liu, Pratip Chakraborty, Joao Pedro Figueira Nunes, Andrew R. Attar, Surjendu Bhattacharyya, Kurtis Borne, Elio Champenois, Nathan Goff, Kareem Hegazy, Matthias C Hoffmann, Fuhao Ji, Ming-Fu Lin, Duan Luo, Lingyu Ma, Asami Odate, Shashank Pathak, Daniel Rolles, Artem Rudenko, Sajib Kumar Saha, Xiaozhe Shen, Xijie Wang, Matthew R Ware, Stephen Weathersby, Peter Weber, Kyle J Wilkin, Thomas J. A. Wolf, Yanwei Xiong, Xuan Xu, Jie Yang, Spiridoula Matsika, Thomas Weinacht, Martin Centurion, *Phys. Chem. Chem. Phys.*, **27**, 471-480, (2025) https://doi.org/10.1039/D4CP02785J
7. "Modeling the Effect of Substituents on the Electronically Excited States of Indole Derivatives", J. Howe, S. Abou-Hatab, S. Matsika, *J. Comput. Chem.*, **46**, e27502, (2025) https://doi.org/10.1002/jcc.27502
8. "Detecting Centrosymmetric Molecular Ions at an Interface with Vibrational Sum Frequency Generation Spectroscopy" Authors: Mandal, Bijoya; Dadashi, Somaiyeh; Kumagai, Koichi; Hirano, Tomonori; Ishiyama, Tatsuya; Abou-Hatab, Salsabil; Zou, Yunqian; Matsika, Spiridoula; Morita, Akihiro; Borguet, Eric, *J. Phys. Chem. C*, **128**, 50, 21508–21517, (2024) https://pubs.acs.org/doi/10.1021/acs.jpcc.4c05318
9. "Exploring Electronic Resonances in Pyridine: Insights from Orbital Stabilization Techniques" Maneesh Pyla and Spiridoula Matsika, *J. Chem. Phys.*, **161**, 154306, (2024) https://doi.org/10.1063/5.0232581
10. "Spectroscopic approaches for studies of site-specific DNA base and backbone 'breathing' using exciton-coupled dimer-labeled DNA", Andrew H. Marcus, Spiridoula Matsika, Dylan Heussman,

Mohammed I. Sorour, Jack Maurer, Claire S. Albrecht, Lulu Enkhbaatar, Patrick Herbert, Kurt A. Kistler and Peter H. von Hippel, chapter for volume: Nucleic Acid Photophysics and Photochemistry, in book series, "Nucleic Acids and Molecular Biology", vol. 36, page 157-209, Springer, 2024 https://doi.org/10.1007/978-3-031-68807-2_7

11. "Molecular Dynamical and Quantum Mechanical Exploration of the Site-Specific Dynamics of Cy3 dimers internally linked to dsDNA", Mohammed I. Sorour, Kurt A. Kistler, Andrew H. Marcus, and Spiridoula Matsika, *J. Phys. Rev. B*, **128**, 7750-7760, (2024)
12. "Quantum contributions to Coulomb-explosion imaging revealed by trajectory-surface-hopping molecular dynamics", Singh,Vaibhav, Cheng,Chuan, Weinacht,Thomas, Matsika, Spiridoula, *Phys. Rev. A*, **109**, 052813 , (2024) https://doi.org/10.1103/PhysRevA.00.002800
13. "Time-Resolved Photoelectron Spectroscopy via Trajectory Surface Hopping", Pratip Chakraborty, Spiridoula Matsika, Wiley Interdiscip. Rev. Comput. Mol. Sci., 14, e1715, (2024) http://dx.doi.org/10.1002/wcms.1715
14. "Excited State Hydrogen or Proton Transfer Pathways in microsolvated n-cyanoindole fluorescent probes", Salsabil Abou-Hatab and Spiridoula Matsika, *Phys. Chem. Chem. Phys.*, **26**, 4511-4523, (2024), https://doi.org/10.1039/D3CP04844F
15. "Using transition density models to interpret experimental optical spectra of exciton-coupled cyanine (iCy3)2 dimer probes of local DNA conformations at or near functional protein binding sites", Heussman, Dylan; Enkhbaatar, Lulu; Sorour, Mohammed; Kistler, Kurt; von Hippel, Peter; Matsika, Spiridoula; Marcus, Andrew *Nucleic Acids Research*, 52 , 1272–1289, (2024) https://doi.org/10.1093/nar/gkad1163
16. "Unravelling the Origin of the Vibronic Spectral Signatures in an Excitonically Coupled Indocarbocyanine Cy3 Dimer", Sorour, Mohammed; Marcus, Andrew; Matsika, Spiridoula; *J. Phys. Chem. A*, , **127**, 9530-9540, (2023) https://doi.org/10.1021/acs.jpca.3c06090
17. "Excited State Dynamics of o-Nitrophenol Studied with UV Pump VUV Probe Time Resolved Photoelectron and Photoion Spectroscopy", Samuel McClung, Dakshitha Abeygunewardane, Spiridoula Matsika, and Thomas Weinacht, *J. Chem. Phys.*, **158**, 144303, (2023) https://doi.org/10.1063/5.0146399
18. "Mechanistic aspects of the effect of flanking nucleotide sequence on CPD formation and CPD self-repair in DNA", Lee, Wook; Matsika, Spiridoula, *J. Phys. Chem. B*, **127**, 18-25, (2023)
19. "Spectroscopy and Theoretical Modeling of Tetracene Anion Resonances", Cole R. Sagan, Cate S. Anstöter, Mushir Thodika, Kenneth D. Wilson, Spiridoula Matsika, and Etienne Garand, *J. Phys. Chem. Lett.*, **13**, 10245-10252, (2022) https://doi.org/10.1021/acs.jpclett.2c02931
20. "Effective Fragment Potentials for Microsolvated Excited and Anionic States", Cate S. Anstöter, Salsabil Abou-Hatab, Mushir Thodika, Spiridoula Matsika, *J. Phys. Chem. A*, **126**, 8508-8518, (2022) https://doi.org/10.1021/acs.jpca.2c06122
21. "Strong Field Double Ionization of Formaldehyde Investigated using Momentum Resolved Covariance Imaging and Trajectory Surface Hopping" Chuan Cheng, Vaibhav Singh, Spiridoula Matsika, Thomas Weinacht, *J. Phys. Chem. A*, **126**, 7399-7406, (2022)
22. "Nonadiabatic Excited State Dynamics of Organic Chromophores: Take-home Messages", Pratip Chakraborty, Yusong Liu, Samuel McClung, Thomas Weinacht, and Spiridoula Matsika, *J. Phys. Chem. A*, **126**, 6021-6031, (2022), DOI: 10.1021/acs.jpca.2c04671
23. "Stable Excited Dication: Trapping on the S_1 State of Formaldehyde Dication After Strong Field Ionization" Vaibhav Singh, Chuan Cheng, Thomas Weinacht, Spiridoula Matsika, *Phys. Chem. Chem. Phys.*, **24**, 20701 - 20708, (2022) (2022 hot PCCP article) DOI: 10.1039/D2CP02604J

24. "Developments in ultrafast spectroscopy", Chantal Daniel, Luis Bañares, Spiridoula Matsika, Jin Zhao, *Phys. Chem. Chem. Phys.*, **24**, 12082-12082, (2022)
25. "Modeling the Electronic Absorption Spectra of the Indocarbocyanine Cy3", Mohammed I. Sorour, Andrew H. Marcus, Spiridoula Matsika. *Molecules*, **27**, 4062, (2022) https://doi.org/10.3390/molecules27134062
26. "Conformer-Specific Dissociation Dynamics in Dimethyl Methylphosphonate Radical Cation", Vaibhav Singh, Hugo A. López Pena, Jacob M. Shusterman, Patricia Vindel-Zandbergen, Katharine Moore Tibbetts, Spiridoula Matsika, *Molecules*, **27**, 2269, (2022)
27. "Projected Complex Absorbing Potential Multi-reference Configuration Interaction Approach for Shape and Feshbach Resonances", Mushir Thodika, Spiridoula Matsika, *J. Chem. Theory Comput.*, **18**, 3377, (2022) https://doi.org/10.1021/acs.jctc.1c01310
28. "A unique $\mathcal{QP}$-partitioning and Siegert width using real-valued continuum-remover potential", Y. Sajeev, Mushir Thodika, Spiridoula Matsika, *J. Chem. Theory Comput.*, **18**, 2863-2874, (2022)
29. "Exact-Factorization-Based Surface-Hopping for Multi-State Dynamics", Patricia Vindel Zandbergen, Spiridoula Matsika, and Neepa T. Maitra, *J. Phys. Chem. Lett.*, **13**, 1785, (2022) https://doi.org/10.1021/acs.jpclett.1c04132
30. "2021 Benjamin Franklin Medal in Chemistry presented to Roberto Car, Ph.D. and Michele Parrinello, Ph.D.", *Journal of the Franklin Institute*, Spiridoula Matsika, **358**, 9400, (2021)
31. "Accurate Modeling of Excitonic Coupling in Cyanine Dye Cy3", Mohammed I. Sorour, Kurt A. Kistler, Andrew H. Marcus, and Spiridoula Matsika, *J. Phys. Chem. A*, **125**, 7852 -7866, (2021)
32. "Modeling the Ultrafast Electron Attachment Dynamics of Solvated Uracil", Cate S. Anstöter, Mark DelloStritto, Michael L. Klein, and Spiridoula Matsika, *J. Phys. Chem. A*, **125**, 32, 6995 - 7003, (2021)
33. "Time Resolved Photoelectron Spectroscopy as a Test of Electronic Structure and Nonadiabatic Dynamics", Pratip Chakraborty, Yusong Liu, Samuel McClung, Thomas Weinacht, and Spiridoula Matsika, *J. Phys. Chem. Lett.*, **12**, 5099 - 5104, (2021)
34. "Electronic structure methods for the description of nonadiabatic effects and conical intersections", Spiridoula Matsika *Chem. Rev.*, **121**, 9407 - 9449, (2021)
35. "Modeling Solvation Effects on Absorption and Fluorescence Spectra of Indole in Aqueous Solution", Salsabil Abou-Hatab, Vincenzo Carnevale and Spiridoula Matsika *J. Chem. Phys.*, **154**, 064104 (2021)
36. "Effect of Dynamic Correlation on the Ultrafast Relaxation of Uracil in the Gas Phase", Pratip Chakraborty, Yusong Liu, Thomas Weinacht, and Spiridoula Matsika, *Faraday Discussions*, **228**, 266-285, (2021)
37. "Benchmarking Quantum Mechanical Methods for the Description of Charge-Transfer States in π Stacked Nucleobases" Camilo Zuluaga, Vincent A. Spata, and Spiridoula Matsika, *J. Chem. Theory Comput.*, **17**, 376 - 387, (2021)
38. "Description of Two-particle One-hole Electronic Resonances using Orbital Stabilization Methods" Mushir Thodika, Nathan Mackouse and Spiridoula Matsika, *J. Phys. Chem. A*, **124**, 9011- 9020, (2020)
39. "Understanding the Interplay Between the Non-Valence and Valence State of the Uracil Anion Upon Mono-Hydration", Cate S. Anstöter and Spiridoula Matsika, *J. Phys. Chem. A*, **124**, 9237-9243, (2020)

40. "Stabilization of triplet biradical intermediate of 5-methylcytosine enhances cyclobutane pyrimidine dimer (CPD) formation in DNA" Wook Lee and Spiridoula Matsika *Chemistry- A European Journal*, **26**, 14181-14186, (2020)
41. Excited State Dynamics of cis,cis-1,3-Cyclooctadiene: UV Pump VUV Probe Time Resolved Photoelectron Spectroscopy Yusong Liu, Pratip Chakraborty, Spiridoula Matsika and Thomas Weinacht *J. Chem. Phys.*, **153**, 074301, (2020)
42. Excited State Dynamics of cis,cis-1,3-Cyclooctadiene: Non-adiabatic Trajectory Surface Hopping Pratip Chakraborty, Yusong Liu, Thomas Weinacht, and Spiridoula Matsika *J. Chem. Phys.*, **152**, 174302 (2020)
43. "The Generality of the GUGA MRCI Approach in COLUMBUS for Treating Complex Quantum Chemistry", Hans Lischka, Ron Shepard, Thomas Müller, Péter G. Szalay, Russel M. Pitzer, Adelia J. A. Aquino, Mayzza M. Arajo do Nascimento, Mario Barbatti, Lachlan T. Belcher, Itamar Borges Jr., Scott R. Brozell, Anita Das, Silmar A. do Monte, Leticia Gonzalez, William L. Hase, Gary Kedziora, Fabris Kossoski, Francisco B. C. Machado, Spiridoula Matsika, Dana Nachtigallova, Reed Nieman, Markus Oppel, Felix Plasser, Rene F. K. Spada, Eric A. Stahlberg, Elizete Ventura, David R. Yarkony *J. Chem. Phys.*, **152**, 134110, (2020)
44. "Comparative study of methodologies for calculating metastable states of small to medium-sized molecules", Mushir Thodika, Mark Fennimore, Tolga N.V. Karsili, and Spiridoula Matsika, *J. Chem. Phys.*, **151**, 244104, (2019)
45. "Electron correlation in channel resolved strong field molecular double ionization", Chuan Cheng, Patricia Vindel Zandbergen, Spiridoula Matsika, and Thomas Weinacht, *Phys. Rev. A*, **100**, 053405, (2019)
46. "Theoretical Investigation of Positional Substitution and Solvent Effects on n-Cyanoindole Fluorescent Probes", Salsabil Abou-Hatab and Spiridoula Matsika, *J. Phys. Chem. B*, **123**, 7424 - 7435, (2019)
47. "Intersystem crossing in the exit channel ", Hongwei Li, Alexander Kamasah, Spiridoula Matsika, Arthur G. Suits, *Nature Chemistry*, **11**, 123, (2019)
48. "Role of charge transfer states into the formation of cyclobutane pyrimidine dimers in DNA", Wook Lee and Spiridoula Matsika, *Faraday Discussions*, **216**, 507 - 519, (2019)
49. "Ultrafast Photoinduced Processes in Polyatomic Molecules: Electronic Structure, Dynamics and Spectroscopy dedicated to Prof. Wolfgang Domcke on the occasion of his 70th birthday", Maxim F. Gelin, Spiridoula Matsika, Andrzej Sobolewski, Yoshitaka Tanimura *Chem. Phys.*, **515**, 1-2, (2018)
50. "Strong and Weak-Field Ionization in Pump-Probe Spectroscopy", Spencer L. Horton, Yusong Liu, Pratip Chakraborty, Philipp Marquetand, Tamas Rozgonyi, Spiridoula Matsika, and Thomas Weinacht, *Phys. Rev. A*, **98**, 053416, (2018)
51. "The Origin of Fluorescence in DNA Thio-Analogues", Tolga N. V. Karsili, Mushir Thodika, Linh Nguyen, Spiridoula Matsika *Chem. Phys.*, **515**, 434-440, (2018)
52. "Introduction: Theoretical Modeling of Excited State Processes", Spiridoula Matsika and Anna I. Krylov, *Chem. Rev.*, **118**, 6925 - 6926, (2018)
53. "Electron-induced origins of prebiotic sugars: self-reactions of methanol anion clusters", Tolga N.V. Karsili, Mark A. Fennimore, and Spiridoula Matsika, *Phys. Chem. Chem. Phys.*, **20**, 12599 - 12607, (2018)
54. "Quadruple coincidence measurement of electron correlation in strong field molecular double ionization", Arthur Zhao, Chuan Cheng, Spiridoula Matsika and Thomas Weinacht, *Phys. Rev. A*, **97**, 043412, (2018)

55. "Electronic Resonances of Nucleobases Using Stabilization Methods", Mark A. Fennimore, and Spiridoula Matsika, *J. Phys. Chem. A*, **122**, 4048-4057, (2018)
56. "Photochemical Formation of Cyclobutane Pyrimidine Dimers in DNA through electron transfer from a flanking base", Wook Lee and Spiridoula Matsika, *ChemPhysChem*, **19**, 1568-1571, (2018) Correction: *ChemPhysChem*, **20**, 1545, (2019)
57. "Origins of Photodamage in Pheomelanin Constituents: Photochemistry of 4-Hydroxybenzothiazole", Tolga N.V. Karsili, Barbara Marchetti, and Spiridoula Matsika, *J. Phys. Chem. A*, **122**, 1986-1993, (2018)
58. "Calculations of non-adiabatic couplings within equation-of-motion coupled-cluster framework: Theory, implementation, and validation against multi-reference methods", Shirin Faraji, Spiridoula Matsika, and Anna I. Krylov, *J. Chem. Phys*, **148**, 044103, (2018)
59. "Mechanistic insights into photoinduced damage of DNA and RNA nucleobases in the gas phase and in bulk solution", Pratip Chakraborty, Tolga N.V. Karsili, Barbara Marchetti, and Spiridoula Matsika, *Faraday Discussions*, **207**, 329 - 350, (2018)
60. "Vibrationally Assisted Below Threshold Ionization", Spencer L. Horton, Yusong Liu, Pratip Chakraborty, Spiridoula Matsika, and Thomas Weinacht, *Phys. Rev. A*, **95**, 063413, (2017)
61. "Mechanisms of H and CO Loss from the Uracil Anion Following Low Energy Electron Irradiation", Mark A. Fennimore, Tolga N. V. Karsili and Spiridoula Matsika, *Phys.Chem.Chem.Phys.*, **19**, 17233 - 17241, (2017)
62. "Controlling Photorelaxation in Uracil with Shaped Laser Pulses: A Theoretical Assessment", Keefer, Daniel; Thallmair, Sebastian; Matsika, Spiridoula; de Vivie-Riedle, Regina, *J.Am. Chem. Soc.*, **139**, 5061 - 5066, (2017)
63. "Ultrafast Internal Conversion Dynamics of Highly Excited Pyrrole Studied with VUV/UV Pump Probe Spectroscopy", Spencer L. Horton, Yusong Liu, Pratip Chakraborty, Spiridoula Matsika, and Thomas Weinacht, *J. Chem. Phys.*, **146**, 064306 (2017)
64. "Substituent Effects on the Absorption and Fluorescence Properties of Anthracene", Salsabil Abou-Hatab, Vincent A. Spata, Spiridoula Matsika, *J. Phys. Chem. A*, **121**, 1213 - 1222, (2017)
65. "Conformational and electronic effects on the formation of anti cyclobutane pyrimidine dimer in G-quadruplex structure", Wook Lee and Spiridoula Matsika, *Phys.Chem.Chem.Phys.*, **19**, 3325 - 3336, (2017)
66. "Core-Excited and Shape Resonances of Uracil", Mark A. Fennimore and Spiridoula Matsika, *Phys.Chem.Chem.Phys.*, **18**, 30536 - 30545, (2016) Correction: *Phys.Chem.Chem.Phys.*, **19**, 29005 - 29006, (2017)
67. "Photophysical Properties of Pyrrolocytosine, a Cytosine Fluorescent Base Analogue", Nguyen, Quynh, Vincent A. Spata, Spiridoula Matsika, *Phys.Chem.Chem.Phys.*, **18**, 20189 - 20198, (2016)
68. "Coexistence of different electron transfer mechanisms in the DNA repair process by photolyase", Wook Lee, Goutham Kodali, Robert J. Stanley, Spiridoula Matsika, *Chemistry-A European Journal*, **22**, 11371-11381, (2016)
69. "Molecular Double Ionization using Strong Field Few Cycle Laser Pulses", Arthur Zhao, Péter Sándor, Vincent Tagliamonti, Thomas Weinacht, and Spiridoula Matsika, *J. Phys. Chem. A*, **120**, 3233 - 3240, (2016)
70. "Excimers and Exciplexes in Photoinitiated Processes of Oligonucleotides", Vincent A. Spata, Wook Lee and Spiridoula Matsika, *J. Phys. Chem. Lett.*, invited perspective, **7**, 976 - 984, (2016)

71. "Surface hopping investigation of the relaxation dynamics in radical cations", Mariana Assmann, Thomas Weinacht, and Spiridoula Matsika, *J. Chem. Phys.*, **144**, 034301 (2016)

72. "Photophysical Deactivation Pathways in Adenine Oligonucleotides", Vincent A. Spata and Spiridoula Matsika, *Phys.Chem.Chem.Phys.*, **17**, 31073, (2015)

73. "Controlling the Dissociation Dynamics of Acetophenone Radical Cation Through Excitation of Ground and Excited State Wavepackets", Moore Tibbetts, Katherine; Tarazkar, Maryam; Bohinski, Timothy; Romanov, Dmitri; Matsika, Spiridoula; Levis, Robert; *Journal of Physics B: Atomic, Molecular and Optical Physics*, **48**, 164002, (2015)

74. "Excited state relaxation of neutral and basic 8-Oxoguanine", Zhen Lu, Ashley Beckstead, Bern Kohler, Spiridoula Matsika, *J. Phys. Chem. B*, **119**, 8293 - 8301, (2015); "Correction to "Excited State Relaxation of Neutral and Basic 8-Oxoguanine" *J. Phys. Chem. B*, **120**, 597-597, (2016)

75. "QM/MM studies reveal pathways leading to the quenching of the formation of thymine dimer photoproduct by flanking bases", Wook Lee and Spiridoula Matsika, *Phys.Chem.Chem.Phys.*, **17**, 9927 - 9935, (2015)

76. "Photoelectron spectrum and dynamics of the uracil cation", Mariana Assmann, Horst Köppel and Spiridoula Matsika, *J. Phys. Chem. A*, **119**, 866 - 875, (2015)

77. "Modified Nucleobases', S. Matsika, "Topics in Current Chemistry - Photoinduced Phenomena in Nucleic Acids", **355**, 209-243, (2015)

78. "Strong Field Adiabatic Ionization Prepares a Launch State for Coherent Control", Timothy Bohinski; Katharine Moore Tibbetts; Maryam Tarazkar; Dmitri Romanov; Spiridoula Matsika; Robert Levis, *J. Phys. Chem. Lett.*, **5**, 4305 - 4309, (2014)

79. "Tribute to David R. Yarkony", Spiridoula Matsika, Henry F. Schaefer, III, and Michael S. Schuurman, *J. Phys. Chem. A*, **118**, 11837 - 11837, (2014)

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81. "Role of Excitonic Coupling and Charge-Transfer States in the Absorption and CD Spectra of Adenine-Based Oligonucleotides Investigated through QM/MM Simulations", Vincent A. Spata and Spiridoula Matsika *J. Phys. Chem. A*, **118**, 12021-12030, (2014)

82. "Theoretical Studies of the Excited States of p-Cyanophenylalanine and Comparisons with the Natural Amino Acids Phenylalanine and Tyrosine", Stephen Meloni and Spiridoula Matsika; *Theoretical Chemistry Accounts*, **133**, 1497, (2014) (invited article in honor of S. Shavitt)

83. "Radical Cation Spectroscopy of Substituted Alkyl Phenyl Ketones via Tunnel Ionization", Timothy Bohinski; Katharine Moore Tibbetts; Kristin Munkerup; Maryam Tarazkar; Dmitri Romanov; Spiridoula Matsika; Robert Levis, *Chemical Physics*, **442**, 81-85, (2014)

84. "Ultrafast Excited-State Dynamics and Vibrational Cooling of 8-oxo-7,8-dihydro-2-deoxyguanosine in D_2O", Zhang, Yuyuan; Dood, Jordan; Beckstead, Ashley; Chen, Jinquan; Li, Xibo; Burrows, Cynthia; Lu, Zhen; Matsika, Spiridoula; Kohler, Bern, *J. Phys. Chem. A*, **117**, 12851-12857, (2013)

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86. "Ultrafast Relaxation Dynamics of Uracil Probed via Strong Field Dissociative Ionization", S. Matsika, M. Spanner, M. Kotur, and T. Weinacht, *J. Phys. Chem. A*, **117**, 12796 - 12801, (2013)

87. "Excited-State Tautomerization of Gas-Phase Cytosine", C. G. Triandafillou and S. Matsika, *J. Phys. Chem. A*, **117**, 12165-12174, (2013) (invited article for the Curt Wittig Festschrift)

88. "Dissociative electron attachment to carbon dioxide via the $^2\Pi_u$ shape resonance", A. Moradmand, D. S. Slaughter, D. J. Haxton, T. N. Rescigno, C. W. McCurdy, T. Weber, S. Matsika, A. L. Landers, A. Belkacem, and M. Fogle, *Phys. Rev. A*, **88**, 032703, (2013)

89. "Bonded Excimer Formation in π-Stacked 9-Methyladenine Dimers", V. A. Spata and S. Matsika, *J. Phys. Chem. A*, **117**, 8718-8728, (2013) (invited article for Special Section for the Structure and Dynamics: Born - Oppenheimer Theories and Applications, Reaction Dynamics and Molecule Surface Scattering)

90. "High-Multiplicity Natural Orbitals in Multireference Configuration Interaction for Excited State Potential Energy Surfaces", Z. Lu and S. Matsika, *J. Phys. Chem. A*, **117**, 7421 - 7430, (2013) (invited article for the Joel M. Bowman Festschrift)

91. "Exciplexes and conical intersections lead to fluorescence quenching in π-stacked dimers of 2-aminopurine with purine nucleobases", J.X. Liang, Q. Nguyen and S. Matsika, *Photochemical & Photobiological Sciences*, **12**, 1387-1400, (2013) (invited article for special issue on "Interaction of UV radiation with DNA")

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94. "Ultrafast Excited State Dynamics of Allopurinol, a Modified DNA Base", J. P. Villabona-Monsalve, R. E. Islas, W. Rodríguez-Córdoba, S. Matsika and J. Peón, *J. Phys. Chem. A*, **117**, 898-890, (2013)

95. "A benchmark of excitonic couplings derived from atomic transition charges", K. A. Kistler, F.C. Spano and S. Matsika, *J. Phys. Chem. B*, **117**, 2032-2044, (2013)

96. "Contrasting Photophysical Behaviors of Star-shaped vs Linear Chromophores", C. M. Pochas, K. A. Kistler, H. Yamagata, S. Matsika and F.C. Spano, *J. Am. Chem. Soc.*, **135**, 3056-3066, (2013)

97. "Final State Distributions in Strong Field Molecular Ionization", M. Kotur, C. Zhou, S. Matsika, S. Patchkovskii, M. Spanner, and T. C. Weinacht, *Phys. Rev. Lett.*, **109**, 203007, (2012)

98. "Dyson norms in XUV and strong-field ionization of polyatomics: Cytosine and uracil", M. Spanner, S. Patchkovskii, C. Zhou, S. Matsika, M. Kotur, and T. C. Weinacht, *Phys. Rev. A*, **86**, 053406, (2012)

99. "Fragmentation Pathways in the Uracil Radical Cation", C. Zhou, S. Matsika, M. Kotur and T. Weinacht, *J. Phys. Chem. A*, **116**, 9217-9227, (2012)

100. "The influence of excited state topology on wavepacket delocalization in the relaxation of photoexcited polyatomic molecules", P. Krause, S. Matsika, M. Kotur and T. Weinacht, *J. Chem. Phys.*, **137**, 22A537, (2012) (invited article for the Special Issue on Nonadiabatic Dynamics)

101. "On the Accessibility to Conical Intersections in Purines: Hypoxanthine and its Singly Protonated and Deprotonated Forms", J. Villabona-Monsalve, R. Noria, S. Matsika, J. Peon, *J. Am. Chem. Soc.*, **134**, 7820 - 7829, (2012)

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103. "High-multiplicity natural orbitals in multireference configuration interaction for excited states", Z. Lu and S. Matsika, *J. Chem. Theory Comput.*, **8**, 509-517, (2012)

104. "Nuclear Dynamics on a Three-state Jahn-Teller Model System", P. Krause and S. Matsika, *J. Chem. Phys.*, **136**, 034110 (2012)

105. "Absorption, Circular Dichroism and Photoluminescence in Perylene Diimide Bichromophores: Polarization Dependent H- and J-aggregate Behavior", K. A. Kistler, C. M. Pochas, H. Yamagata, S. Matsika and F.C. Spano, *J. Phys. Chem. B*, **116**, 77 - 86, (2012)

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156. "Ab Initio Study of the Ground and Several Excited States of the NLi System", S. Matsika, A. Papakondylis and A. Mavridis, *Chem. Phys. Lett.*, **250**, 409-414, (1996)

INVITED TALKS AT CONFERENCES AND WORKSHOPS (108 total)

1. Fall 2025 DCP Frontiers in Chemical Physics seminar series, November 14, 2025
2. "Solvation effects on photochemical and electron driven processes", Core-to-core symposium UCSB-JSPS "Elucidation of solvation effects on molecular recognition", Santa Barbara, September 15-17, 2025,
3. "Modeling Ultrafast Excited State Dynamics", XXIX Dynamics of Molecular Collisions, Snowbird, UT, July 6-11, 2025
4. "Insights into ultrafast excited state dynamics by combining theory and experiment", DAMOP 2025, Portland, OR, June 16-20, 2025
5. "Theoretical insights into electron induced processes in organic molecules", 20th Spectroscopy and Dynamics of Molecules and Clusters (SDMC) Conference,, India, February 20 to 23, 2025
6. "Modeling Pump-Probe Experiments to Reveal Nonadiabatic Dynamics of Polyatomic Molecules", Theories and Computational Methods for Accurate and Efficient Calculation of Electronic Transitions and Spectroscopy, NYC, December 6, 2024
7. "Combining trajectory surface hopping with pump-probe spectroscopies to understand nonadiabatic dynamics of polyatomic molecules", AMOS DOE meeting October 2024
8. "Metastable anions in gas and condensed phases", Telluride workshop on "Advances in Theory of Electronic Resonances", July 15-20, 2024
9. "Modeling experimental observables", Telluride workshop on Spectroscopy and Dynamics on Multiple Potential Energy Surfaces, Telluride, July 21-26, 2024
10. "Combining theory and experiment to reveal nonadiabatic dynamics", 24th European Conference on the Dynamics of Molecular Systems (MOLEC), Aarhus, Denmark, June 30-July 5, 2024
11. "Theoretical modeling of experimental observables to study nonadiabatic dynamics", GRC on "Multidimensional Imaging of Chemical Dynamics", Bryant University, RI, June 9-14, 2024
12. "Modeling pump-probe spectroscopies from excited state dynamics", 25 years of PCCP , Amsterdam, Netherlands, April 30-May 3, 2024
13. "Nonadiabatic events in photon and electron driven processes", Conference: The Path of Quantum Chemistry into the 21st Century, ETH Zurich, January 16-18, 2024
14. "Theoretical description of nonadiabatic events in photon and electron driven processes", ACS, San Francisco, August 13-17, 2023
15. "Theoretical description of electron induced processes in DNA building blocks", POSMOL 2023, University of Notre Dame, Indiana, USA, August 3-6, 2023
16. "Modeling Experimental Observables from Excited State Dynamics", ICQC2023, Bratislava, June 2023
17. "Theoretical description of nonadiabatic events in photon and electron driven processes", CECAM workshop on "Triggering out-of-equilibrium dynamics in molecular systems", Lausanne, Switzerland, March 28-31, 2023

18. "Theoretical description of nonadiabatic events in photon and electron driven processes", Symposium of Theoretical Chemistry, Heidelberg, Germany, September 18-22, 2022
19. "Theoretical description of nonadiabatic events in photon and electron driven processes", WATOC 2022, Vancouver, July 2022
20. "Quantum chemistry applied to electron driven processes", Molecular Quantum Mechanics (MQM) 2022, June 2022, Blacksburg, Virginia
21. "Combining theory and experiment to observe excited state dynamics in organic chromophores", National ACS meeting, March 20, 2022
22. "Theoretical modeling of electronically excited states and their spectroscopic signatures in biological systems", Pacifichem 2021, December 19, 2021
23. "Electron attachment to solvated nucleobases", Pacifichem 2021, December 18, 2021
24. "Exploring nonadiabatic dynamics in organic chromophores", online Seminar Series on "Theory and Simulation of Electronic and Optical Processes in Molecules and Materials", December 8, 2021
25. "Using multiconfigurational methods to interpret photon and electron driven processes in molecular systems", National ACS meeting, August 2021
26. "Modeling Photophysics and Photochemistry in Organic and Biological Molecules", International Conference on Photochemistry (ICP) 19-23 July, 2021
27. "Comparing different theoretical approaches to describe shape and Feshbach resonances", Telluride workshop on "Advances in Theory of Electronic Resonances", July 2021
28. "Exploring nonadiabatic dynamics by modeling experimental observables", Telluride workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", July 2021
29. "Fighting Bias, Stereotypes, Imposter Syndrome, and Trying to Achieve a Family-Work Balance", Younger Chemist Committee, Global Women Breakfast 2021
30. "Effect of Dynamic Correlation on the Ultrafast Relaxation of Uracil in the Gas Phase", Faraday Discussions, February 2-4, 2021
31. "Quantum chemistry applied to electron driven processes", Lowdin Symposium 2020, December 3-4, 2020
32. "Modeling photophysics and photochemistry in complex systems ", ACS Meeting, August 18th, 2020
33. "Conical intersections and non adiabatic dynamics in conjugated molecules", Telluride Science Summer Lecture Series: XXVth International Symposium on the Jahn-Teller Effect, July 20, 2020
34. "Unraveling excited state dynamics and spectroscopy in organic chromophores", 2020 Pacific Conference on Spectroscopy and Dynamics, San Diego CA, Jan 30-Feb 2, 2020
35. "Using computers, physics and mathematics to understand chemistry and biology", APS Conference for Undergraduate Women in Physics, January 2020, Temple University
36. "Theoretical approaches to calculating resonances", Telluride workshop on "Advances in Theory of Electronic Resonances", July 22-26, 2019
37. "Nonadiabatic dynamics in photon and electron driven processes", Telluride workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", July 16-20, 2019
38. "Exploring Excited State Potential Energy Surfaces for Photon and Electron Driven Processes", Dynamics of Molecular Collisions, Montana, July 7-12, 2019
39. "Role of charge transfer states into the formation of cyclobutane pyrimidine dimers in DNA", Faraday Discussion on "Ultrafast Photoinduced Energy and Charge Transfer", Ventura, CA, April 8-10, 2019
40. "Modeling Photophysics and Photochemistry in Complex Systems", "Chemistry and Physics of Advanced Materials - III" symposium at IISER Pune, India, October 2018

41. “Employing electronic structure and dynamics calculations to interpret weak and strong field ionization pump probe experiments ”, 256th ACS National Meeting in Boston, MA, August 19-23, 2018
42. ”Theoretical description of nonadiabatic events in photon and electron driven processes”, 256th ACS National Meeting in Boston, MA, August 19-23, 2018
43. ”Nonadiabatic events in photon and electron driven processes”, Telluride Workshop on “Spectroscopy and Dynamics on Multiple Surfaces”, Telluride, CO, July 2018
44. ”Nonadiabatic Effects in Photon and Electron Driven Reactions”, Molecular Interactions and Dynamics Gordon Research Conference, Easton, MA, July 8-13, 2018
45. “Theoretical studies of photochemistry in nucleic acids”, ASP 2018 Biennial Meeting, Tampa, FL, 12-15 May 2018
46. “Nonadiabatic Dynamics in Condensed Phases”, Gordon Conference on Molecular and Ionic Clusters, February 25- March 2, 2018, Italy
47. “Theoretical Studies of the Interaction of Uracil with Low Energy Electrons”, 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany, August 27 - September 1, 2017
48. “Theoretical insight into the photophysics and photochemistry related to DNA damage and repair”, 13th Femtochemistry conference, Cancun, Mexico, August 12-17, 2017
49. “ Interaction of nucleobases with low energy electrons”, Telluride workshop on ”Photo Physics of Biomolecular Ions”, July, 2017
50. “ Photophysics and photochemistry in oligonucleotides”, Telluride workshop on ”Photo Physics of Biomolecular Ions”, July 24-28, 2017
51. “Resonances and Dissociative Electron Attachment in Uracil using Stabilization Methods”, Telluride workshop on ”Advances in theory of electronic resonances”, July 17-21, 2017
52. “ Insights into the nonadiabatic dynamics of radical cations”, APS March Meeting, New Orleans, March 13-17, 2017
53. “QM/MM studies of photophysics and photochemistry related to DNA damage and repair”, 26th Inter-American Photochemical Society Meeting Sarasota, FL, January 2-5, 2017
54. “QM/MM Studies of Photoinitiated Processes in Complex Systems ”,New York Theoretical and Computational Chemistry Conference, NYU, Dec. 2, 2016.
55. “QM/MM Studies of Photoinitiated Processes in Complex Systems”, Penn Conference on Theoretical Chemistry, August 2016.
56. “QM/MM Studies of Photoinitiated Processes in Complex Systems”, ISTCP (International Symposium of Theoretical Chemical Physics), North Dakota, July 2016
57. “Excimers, Exciplexes and Conical Intersections in Photoinitiated Processes of Biological Systems”, Telluride workshop on ”Non-equilibrium Statistical Physics: from molecular materials to theoretical engineering”, July 2016
58. “QM/MM studies of excited states in complex systems”, Pacifichem, Honolulu, HI, December 2015
59. “Obtaining insights into the dynamics of radical cations produced via strong field ionization ”, Pacifichem, Honolulu, HI, December 2015
60. “Combining High Level Ab Initio Calculations with Laser Control of Molecular Dynamics”, AMOS DOE meeting, October 2015
61. “Nonadiabatic events in photoinitiated processes in molecules”, Dynamics of Molecular Collisions, Asilomar, CA, July 2015
62. “Nonadiabatic Dynamics in the Photophysics and Photochemistry of DNA ”, 98th Canadian Chemistry Conference and Exhibition, Ottawa, Canada, June 2015

63. "Insights into the role of excimers/exciplexes in the photophysics and photochemistry of DNA", 249th American Chemical Society meeting in Denver, CO, March 2015
64. "Excimers, charge-transfer states, and conical intersections in the photophysics of oligonucleotides", Telluride Workshop on "Spectroscopy and Dynamics on Multiple Surfaces", Telluride, CO, July 2014
65. "Exciplexes and conical intersections in π-stacked bases in DNA", Workshop on "Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", Telluride, CO, July 2013
66. Introduction to the Non-adiabatic Dynamics Session, Dynamics of Molecular Collisions, Granlibaken CA, July 2013
67. "Exciplexes and Conical Intersections in π-Stacked Dimers of Nucleobases", Workshop on "Advances In Photoreactions: When Spin-Orbit Coupling, Optical Excitation, and Motion of Nuclei are of Equal Importance?", Telluride, CO, June 2013
68. "Exploring nonadiabatic events with strong field molecular ionization", Gordon Research Conference on Molecular Energy Transfer, Vendura, CA, January 2013
69. "Nuclear Dynamics of Model Systems with Two and Three-State Conical Intersections", XXIst International Symposium on the Jahn-Teller Effect, Tsukuba, Japan, August 2012
70. "Theoretical developments for modeling excited states and conical intersections", 244th American Chemical Society meeting in Philadelphia, PA, August 2012
71. "Introduction to the Excited State Dynamics session", Gordon Research Conference on Electronic Spectroscopy and Dynamics, Bates College, Maine, July 2012
72. "Non-adiabatic events in interacting chromophores", Gordon Research Conference on Atomic and Molecular Interactions, Stonehill College, Easton, MA, July 2012
73. "Theoretical developments for studying excited states and their potential energy surfaces", Telluride Workshop on "Spectroscopy and Dynamics on Multiple Surfaces", July 2012
74. "UV radiation and the building blocks of DNA/RNA: What theoretical studies can tell us", Astrobiology Science Conference 2012, April 2012, Atlanta, GA
75. "Theoretical studies of photophysical events in π-stacked dimers of nucleobases", 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), September 2-8, 2011, Tokyo, Japan
76. "Combining dissociative ionization pump probe spectroscopy and ab initio calculations to explore excited state dynamics involving conical intersections", Faraday Discussion 153: Coherence and Control in Chemistry, July 25-27 2011, Leeds, England
77. "Nonadiabatic events in π-stacked interacting chromophores", Telluride workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", July 5-8, 2011, Telluride, CO
78. "Theoretical studies of photophysical properties in π-stacked nucleobase dimers", 51st Sanibel Symposium, February 25 - March 1, 2011, St. Simons Island, Georgia
79. "Combining high hevel ab initio calculations with laser control of molecular dynamics", Pacifichem, December 15-20, 2010, Honolulu, Hawaii
80. "Theoretical studies of excited electronic states of nucleobase dimers ", Pacifichem, December 15-20, 2010, Honolulu, Hawaii
81. "Theoretical developments for modeling excited states and nonadiabatic effects ", Pacifichem, December 15-20, 2010, Honolulu, Hawaii
82. "Conical intersections in non-isolated chromophores", XX International Symposium on the Jahn-Teller Effect, 16th - 20th August 2010, University of Fribourg, Switzerland
83. "Combining theory and experiment to examine how conical intersections affect dynamics on multiple surfaces", Telluride Workshop on "Spectroscopy and Dynamics on Multiple Surfaces", July 2010

84. "Excited electronic states of nucleobase dimers", 239th ACS National Meeting, March 21-25, 2010, San Francisco, CA
85. "Combining High Level Ab Initio Calculations with Laser Control of Molecular Dynamics", Department of Energy, Basic Energy Sciences, AMOS Research Meeting, Airie Conference Center, VA, September 2009
86. "Excited states and conical intersections in non-isolated chromophores", 238th National ACS Meeting, Washington DC, August 2009
87. "The role of conical intersections in the photophysics of biologically relevant molecules", Gordon Conference on Electronic Spectroscopy and Dynamics, Colby College, Maine, July 2009
88. "Two- and three-state conical intersections in molecular systems", Department of Energy, Basic Energy Sciences, Combustion (Gas Phase Chemical Physics), May 2009
89. "Non-adiabatic Effects on Excited States of Biomolecules", 237th National ACS Meeting, March 22-26, 2009, Salt Lake City, Utah
90. "Electronically Excited States and Conical Intersections of Complex Systems using High Level Ab Initio Methods", Workshop on Mathematical and Algorithmic Challenges in Electronic Structure Theory, IMA, University of Minnesota, September 29 - October 3, 2008
91. " Two- and three-state conical intersections in polyatomic molecules", XIX International Symposium on the Jahn-Teller Effect: Vibronic Interactions and Orbital Physics in Molecules and in the Condensed Phase, Heidelberg, Germany, August 2008
92. "Couplings of excited states within and between nucleic acid bases". Telluride Workshop on "Spectroscopy and Dynamics on Multiple Surfaces", July 2008
93. "Theoretical aspects of the photophysical behavior of natural nucleobases and their analogs", 90th Canadian Chemistry: Conference and Exhibition, Alberta, May 24 to May 28, 2008
94. "Exploring two- and three-state conical intersections between electronic states of molecular systems", 48th Sanibel Symposium, February 2008
95. "Non-adiabatic Effects on Excited States of Biomolecules: Photophysics of Nucleic Acid Bases", XXI Conference on Dynamics of Molecular Collisions, Santa Fe, NM, July 8-13, 2007
96. "Photophysics of DNA/RNA Bases and their Analogs", 2007 MARM Meeting, Ursinus College, Collegeville, PA, May 17, 2007
97. "Electronically Excited States and Conical Intersections in Cytosine and its Analogs", 2007 APS March Meeting, Denver, CO, March 5-9, 2007
98. "Substituent Effects on the Excited Electronic States of Cytosine Analogs", 54th annual Western Spectroscopy Association Conference, Asilomar, CA, January 31-February 2, 2007.
99. "Electronically Excited States and Conical Intersections of Complex Systems using High Level Ab Initio Methods", International Conference of Computational Methods in Sciences and Engineering, Crete, Greece, October 2006
100. 2006 Summer School on Computational Materials Science "Ab Initio Molecular Dynamics Simulation Methods in Chemistry" "Electronic Structure for Excited Electronic States" and "Conical Intersections", The Material Computation Center, University of Illinois at Urbana-Champaign, July 31 - August 11, 2006
101. "The Role of Two- and Three-State Conical Intersections in the Photophysical Properties of Pyrimidine Bases", Workshop on 'Spectroscopy and dynamics on multiple surfaces, Telluride; July 2006
102. "Photophysical Properties of Pyrimidine Bases", 17th Inter-American Photochemical Society Conference, Salvador, Bahia, Brazil, June 2006

103. "Determination of Electronically Excited States and Conical Intersections by High Level Ab Initio Methods", 21^{th} Austin Symposium on Molecular Structure, March 2006
104. "Role of Two- and Three-State Conical Intersections in the Photophysics of DNA and RNA Bases", Pacifichem, Honolulu, Hawaii, December 2005
105. "Two- and Three-State Conical Intersections in Complex Systems" 230th ACS National Meeting, August 2005, Washington, DC; Paper PHYS 181.
106. "A Hybrid QM/MM Approach Using Ab Initio MRCI Wavefunctions" workshop on COLUMBUS, Argonne National Laboratory, Chicago, IL, August 2005
107. "Two-state and Three-state Conical Intersections Affecting the Spectroscopy and Dynamics of Radicals", Telluride workshop on Dynamics of Atmospheric Radicals,Telluride; July 2004
108. "Actinyl Ions and the Effect of Ligands on Their Spectra", Relativistic Effects in Heavy-Element Chemistry and Physics, Kerkrade, Netherlands; 21-26 April, 2001.

INVITED TALKS AT UNIVERSITIES (70 total)

1. "Exploring excited state dynamics and spectroscopy using quantum chemistry", Seminar at the Ohio State University, November 10, 2025
2. "Modeling photon and electron driven damage in the building blocks of nucleic acids", IIT-Bombay, India, February 19, 2025
3. "Theoretical insights into photon and electron induced processes in the building blocks of nucleic acids", TIFR, India, February 17, 2025
4. "Understanding Radiation Damage in Biological Systems using Quantum Chemistry ", Bryn Mawr College, April 5, 2024
5. "Modeling absorption spectra in complex environments", University of Heidelberg, January 19, 2024
6. "Modeling photon and electron driven damage in the building blocks of nucleic acids", Penn State, November 9, 2023
7. "Modeling photon and electron driven damage in the building blocks of nucleic acids", Rowan University, February 1, 2023
8. "Modeling photon and electron driven damage in the building blocks of nucleic acids", University of Delaware, November 3, 2022
9. "Modeling photon and electron driven damage in the building blocks of nucleic acids", University of South Dakota, March 7, 2022
10. "Conical intersections in quantum chemistry", Texas A&M University, Department of Mathematics, December 10, 2021
11. "Unraveling excited state dynamics and spectroscopy in organic chromophores", University of Sao Paulo (virtual), March 26, 2021
12. "Modeling Photophysics and Photochemistry in Biological Molecules", University of Oregon, February 8, 2021
13. "Using Hermitian and Non Hermitian Quantum Mechanics to Understand Molecular Reactivity", Department of Mathematics, Temple University, January 2020
14. "Modeling Photophysics and Photochemistry in Complex Systems", TIFR, India, October 2018
15. "Modeling Photochemistry and Electron Driven Chemistry", Texas A&M, September 25, 2018
16. "Modeling photophysics and photochemistry related to DNA damage", Villanova University, March 23, 2018
17. "Nonadiabatic events in photoinitiated processes in molecules", Stony Brook University, March 23, 2017

18. "Modeling Photophysics and Photochemistry in Biological Molecules", University of Southern California, Los Angeles, CA, February 13, 2017
19. "Modeling Photophysics and Photochemistry in Biological Molecules", UC Boulder, CO, November 11, 2016
20. "Modeling photoinitiated processes related to DNA damage", Bowling Green State University, February 24, 2016
21. "Photophysics and photochemistry related to DNA damage", University of Kansas, October 16, 2015
22. "Photoinitiated processes in biologically relevant molecules", Department of Physics, Temple University, September 14, 2015
23. "Modeling Photophysics and Photochemistry in Biological Molecules", Johns Hopkins University, April 7, 2015
24. "Investigating photoinduced processes in biologically relevant molecules", Wayne State University, November 12, 2014
25. "Exploring nonadiabatic events in photoinitiated processes in molecules", Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, June 20, 2014
26. "Photoinitiated processes in biologically relevant molecules", Iowa State University, January 31, 2014
27. "Using quantum chemistry and strong field dissociative ionization pump-probe spectroscopy to investigate photoinitiated processes in molecules", University of Vienna, December 17, 2013
28. "Using quantum chemistry and strong field dissociative ionization pump-probe spectroscopy to investigate photoinitiated processes in molecules", Technical University of Munich, December 5, 2013
29. "Mechanistical insights into fluorescence properties of DNA chromophores and fluorescent analogs", University of Siena, November 20, 2013
30. "Mechanistical insights into fluorescence properties of DNA chromophores and fluorescent analogs", ICCOM U.O.S. di Pisa, November 19, 2013
31. "Mechanistical insights into fluorescence properties of DNA chromophores and fluorescent analogs", Ludwig Maximilians- University of Munich, November 13, 2013
32. "Using quantum chemistry and strong field dissociative ionization pump-probe spectroscopy to investigate photoinitiated processes in molecules", Karlsruhe Institute of Technology, November 11, 2013
33. "Investigating photoinitiated processes in biologically relevant molecules", University of Heidelberg, Heidelberg, Germany, October 7, 2013
34. "How Quantum Mechanics explains the photostability of DNA under UV radiation", National and Kapodistrian University of Athens, Greece, May 20, 2013
35. "How Quantum Mechanics explains the photostability of DNA under UV radiation", University of Ioannina, Greece, May 28, 2013
36. "Theoretical studies of photoinitiated processes in biologically relevant molecules", University of Wisconsin-Madison, April 15, 2013
37. "Quantum chemical studies of photoinitiated events in biological molecules", Löwdin Lectures 2012, Uppsala University, November 23, 2012
38. "What molecules do when they get excited", Löwdin Lectures 2012, Uppsala University, November 22, 2012
39. "Modeling photophysics and photochemistry in biological molecules", University of Louisville, October 19, 2012
40. "Photophysical properties of biologically relevant molecules: A theoretical look", Drexel University, March 8, 2012

41. "The role of conical intersections in photoinitiated processes of biologically relevant molecules", University of California, Davis, January 24, 2012
42. "The role of conical intersections in photoinitiated processes of biologically relevant molecules", Lawrence Berkeley National Laboratory, January 23, 2012
43. " Modeling photoinitiated processes in DNA", Institute for Molecular Science, Okazaki, Japan, September 9, 2011
44. "Conical Intersections in Photoinitiated Processes", CST 10th Anniversary Celebration, Temple University, November 19, 2008
45. "The role of conical intersections in the photophysics of DNA/RNA bases and their analogs", seminar at the University of Pennsylvania, October 2, 2008
46. "The role of conical intersections in the photophysics of DNA/RNA bases and their analogs", seminar at the University of Colorado at Boulder, September 19, 2008
47. "Theoretical insight into the interaction of light with DNA", seminar at Widener University, March 2008
48. "Photophysics of natural nucleobases and their analogs: turning the fluorescence on", seminar at the University of Minnesota, MN, November 7, 2007
49. "Theoretical aspects of the photophysical behavior of natural nucleobases and their analogs", seminar at The Ohio State University, Columbus, OH, November 5, 2007
50. "Photophysical Behavior and Photostability in DNA and RNA bases", seminar at Bryn Mawr, Philadelphia, PA, March 2, 2007.
51. "Photophysical Behavior and Photostability in DNA and RNA bases", seminar at the University of the Sciences in Philadelphia, Philadelphia, PA, January 29, 2007.
52. "Photophysical Behavior and Photostability in DNA and RNA bases" seminar at Florida International University, Miami, Florida, October 2006
53. "Nonadiabatic Photoinitiated Processes through Potential Energy Surface Crossings", seminar at SUNY at Stony Brook, April 2006
54. "Conical Intersections in Photochemistry and Photophysics", seminar at Los Alamos National Laboratory, Los Alamos, NM, October 2005
55. "Understanding Photoinitiated Processes through Potential Energy Surface Crossings" seminar at University of Southern California, Los Angeles, CA, October 2005
56. "Solving the Schrödinger Equation to Understand the Photostability of Biomolecules" seminar at the Department of Mathematics, Temple University, Philadelphia; April 2005
57. "Nonadiabatic Photoinitiated Processes and Photostability in Nucleobases", seminar at Johns Hopkins University, Maryland; February 2005
58. "Photoinitiated Processes in Chemistry and Biology: What do Potential Energy Surface Crossings Tell us about them", seminar at Shippensburg University, Pennsylvania; October 2004
59. "What do Conical Intersections have to do with Chemistry" seminar at the Department of Mathematics, Temple University, Philadelphia; March 2004
60. "Degenerate States in Chemistry", seminar at the Department of Physics, Temple University, Philadelphia; February 2004
61. "Photoinitiated processes in chemistry and biology: What do potential energy surface crossings tell us about them", seminar at Old Dominion University, Norfolk, Virginia; October 2003
62. "Conical Intersections: Understanding Nonadiabatic Reactions in the Atmosphere, Photodissociation of Radicals, and Beyond", University of Memphis, Memphis, Tennessee, December 2002

63. "Conical Intersections: Understanding Nonadiabatic Reactions in the Atmosphere, Photodissociation of Radicals, and Beyond", Tulane University, Louisiana, December 2002
64. "Conical Intersections: Understanding Nonadiabatic Reactions in the Atmosphere, Photodissociation of Radicals, and Beyond", Florida State University, Tallahassee, Florida, November 2002
65. "Conical Intersections in Nonadiabatic Processes", National Institute of Standards and Technology, Gaithersburg, USA; February 2002.
66. "The Role of Conical Intersections in Nonadiabatic Processes", Washington University in St. Louis, St. Louis, USA; January 2002.
67. "Conical Intersections in Nonadiabatic Processes", Indiana University, Bloomington, Indiana, USA; January 2002.
68. "Actinyl Ions and the Effect of Ligands on Their Spectra", seminar at University of Bonn, Bonn, Germany; April 2001.
69. "Actinyl Ions and the Effect of Ligands on Their Spectra: the 5-Fold Way", seminar at Univ. Autonoma Madrid, Madrid, Spain; June 2000.
70. "Actinyl Ions and the Effect of Ligands on Their Spectra: the 5-Fold Way", seminar at Universite P. Sabatier, Toulouse, France; June 2000.

REPRESENTATIVE CONTRIBUTED PRESENTATIONS

1. "Exploring electronic resonances in pyridine: Insights from Orbital Stabilization Techniques", Maneesh Pyla and SM (hot talk presented by MP), Sanibel Symposium, February 2025
2. "Theoretical Insight into the Relaxation Dynamics and Photodissociation Pathways of UV-Excited o-Nitrophenol", Dakshitha Abeygunewardane and SM (poster presented by DA), Sanibel Symposium, February 2025
3. "Strong Field Double Ionization of Formaldehyde", Vaibhav Singh, SM (talk presented by VS), APS DAMOP, June 2023
4. "Excited State Nonadiabatic Dynamics Of o-Nitrophenol: Theoretical Insight into Pump-probe Experiments and Dissociation Mechanisms*", Dakshitha Abeygunewardane, SM (talk presented by DA), APS DAMOP, June 2023
5. "Shape and Feshbach resonances of uracil", 252th American Chemical Society meeting, Philadelphia, PA, August 2016
6. "Dynamics on radical cations governed by conical intersections", March meeting of the American Physical Society, San Antonio, TX, March 2015
7. "Dynamics on radical cations governed by conical intersections", XXII International Symposium on the Jahn-Teller Effect, Austria, August 2014
8. "Bonded Excimer Formation in π-Stacked 9-Methyladenine Dimers", Gordon Research Conference on Photochemistry, Stonehill College, Easton, MA, July 2013 (poster presented by Vincent Spata)
9. "Get excited with High-Multiplicity Natural Orbitals", 244th American Chemical Society meeting, Philadelphia, PA, August 2012, (poster presented by Zhen Lu)
10. "Conical intersections in π-stacked nucleobase dimers containing 2-aminopurine", 244th American Chemical Society meeting, Philadelphia, PA, August 2012, (poster presented by JingXin Liang)

11. "Get excited with High-Multiplicity Natural Orbitals", Gordon Research Conference on Atomic and Molecular Interactions, Stonehill College, Easton, MA, July 2012 (poster presented by Zhen Lu)

12. "Non-adiabatic events in π-stacked chromophores", Gordon Research Conference on Electronic Spectroscopy and Dynamics, Bates College, Maine, July 2012 (poster)

13. "Excited state behavior of stacked nucleobase dimer systems containing 2-aminopurine", 240th American Chemical Society meeting, Boston, PA, August 2010, (poster presented by JingXin Liang)

14. "Excited state coupling of adjacent thymine nucleobases", 237th American Chemical Society meeting, Salt Lake City, 2009, (poster presented by Christopher Kozak)

15. "Three-state conical intersections in cytosine and pyrimidinone bases", 237th American Chemical Society meeting, Salt Lake City, 2009, (presented by Kurt Kistler)

16. "Excited States of Non-isolated Chromophores", 64rd OSU International Symposium on Molecular Spectroscopy, Columbus, OH, June 2009

17. "Three-State Conical Intersections in Biologically Relevant Molecules", 64rd OSU International Symposium on Molecular Spectroscopy, Columbus, OH, June 2009

18. "Three-State Conical Intersections and their Signatures", American Conference on Theoretical Chemistry, Northwestern University, Evanston, IL, July 19-24, 2008 (poster)

19. "Three-state conical intersections in cytosine", 236th American Chemical Society meeting, Philadelphia, 2008, (poster presented by Kurt Kistler)

20. "A Theoretical Study of Substituent Effects on the Excitation Energies of 2-Pyrimidinone and Purine Derivatives", 63rd OSU International Symposium on Molecular Spectroscopy, Columbus, OH, June 2008

21. "Radiationless decay mechanism of cytosine: An ab initio study with comparisons to cytosine analogs", 234th American Chemical Society meeting, Boston, 2007, (presented by Kurt Kistler)

22. "Two- and Three-State Conical Intersections Involved in the Photophysical Properties of Pyrimidine Molecules", 232th ACS National Meeting; San Francisco, CA, September 2006

23. "Two- and Three-State Conical Intersections in Complex Systems", APS meeting; Baltimore, MD, March 2006

24. "Photoinitiated processes in chemistry and biology: What do potential energy surface crossings tell us about them", Muhlenberg College, Allentown, PA; October 2005

25. "Two- and Three-State Conical Intersections in the Photophysics of Nucleic Acid Bases", Conference on the Dynamics of Molecular Collisions; Asilomar, CA, July 2005 (poster)

26. "Radiationless Decay of Excited States in Nucleobases through Conical Intersections", 228th ACS National Meeting, August, 2004, Philadelphia, PA; Paper PHYS 500.

27. "Radiationless Decay of Excited States of Uracil through Conical Intersections", Gordon Research Conference on Atomic and Molecular Interactions, New London, NH, July 2004

28. "Beyond the Two-state Conical Intersections: Three-State Conical Intersections in Radicals ", 226th ACS National Meeting, September 2003, New York, NY; Paper COMP 85.

29. "Beyond the Double Cone: Three-State Conical Intersections in (a) the Allyl Radical (b) the Pyrazolyl Radical", S. Matsika and D. R. Yarkony, XIXth Conference on the Dynamics of Molecular Collisions; Granlibakken Lake Tahoe, CA, July 2003 (poster)

30. "Photodissociation of the Vinoxy Radical through Conical Intersections and Avoided Crossings", S. Matsika and D. R. Yarkony, American Conference on Theoretical Chemistry; Champion, Pennsylvania; July 2002 (poster).

31. "Photodissociation of the Vinoxy Radical through Conical Intersections and Avoided Crossings", S. Matsika and D. R. Yarkony, Gordon Conference: Atomic and Molecular Interactions; Rhode Island; July 2002 (poster).

32. "The Effect of Spin-Orbit Coupling on Conical Intersections", S. Matsika and D. R. Yarkony, Molecular Quantum Mechanics: The Right Answer for the Right Reason; Seattle; Washington; July 2001 (poster).

33. "Conical Intersections in the Presence of Spin-Orbit Coupling", S. Matsika and D. R. Yarkony, 56th Ohio State University International Symposium on Molecular Spectroscopy, June 11-15, 2001; Paper RG11.

34. "Intensities of the Electronic Spectrum of NpO_2^+", S. Matsika and R. M. Pitzer, 55th Ohio State University International Symposium on Molecular Spectroscopy, June , 2000; Paper RH10.

35. "Theoretical Studies of the Electronic Spectra of Actinyl Ions and the Effect of the Surrounding Environment", S. Matsika and R. M. Pitzer, Seminar at Los Alamos National Lab, February 2000.

36. "Theoretical Studies of the Electronic Spectra of Actinyl Ions and the Effect of the Surrounding Environment", S. Matsika and R. M. Pitzer, Seminar at Pacific Northwest National Lab, January 2000.

37. "Actinyl Ions and How the Crystal Environment Affects their Properties", S. Matsika and R. M. Pitzer, Pitzer Memorial Symposium on Theoretical Chemistry, January 9-13, 2000; Berkeley, CA; Poster C65.

38. "Actinyl ions in the Cesium Tetrachlorouranyl Crystal", S. Matsika and R. M. Pitzer, ACS 31st Central Regional Meeting, June 21-23, 1999; Columbus, OH; Poster 348.

39. "Actinyl ions in $Cs_2UO_2Cl_4$ Crystal", S. Matsika and R. M. Pitzer, 54th Ohio State University International Symposium on Molecular Spectroscopy, June 14-18, 1999; Paper RH11.

40. "Ab Initio Calculations of the Neptunyl Ion, NpO_2^{2+}, and of the Dioxoneptunium(+1) Ion, NpO_2^+", S. Matsika and R. M. Pitzer, Relativistic Effects in Heavy-Element Chemistry and Physics, 10-15 April, 1999, Acquafredda di Maratea, Italy; Poster P37.

41. "Ab Initio Calculations of the Neptunyl Ion, NpO_2^{2+}, and of the Dioxoneptunium(+1) Ion, NpO_2^+. Effects of the Crystal Environment", S. Matsika and R. M. Pitzer, 217th National American Chemical Society Meeting, March 21-25, 1999, Anaheim, CA; Paper NUCL 0093.

42. "The Electronic Spectrum of the Neptunyl Ion, NpO_2^{2+} and of NpO_2^+", Computational Chemistry for Nuclear Waste Characterization and Processing: Relativistic Quantum Chemistry of Actinides, Workshop III at Lawrence Berkeley National Lab, September 17-19, 1998.

43. "The Electronic Spectrum of the Neptunyl Ion, NpO_2^{2+}", Computational Chemistry for Nuclear Waste Characterization and Processing: Relativistic Quantum Chemistry of Actinides, Workshop II at Argonne National Lab, January 17-19, 1998.

44. "The Electronic Spectrum of the Neptunyl Ion, NpO_2^{2+} and of NpO_2^{+}", The National and Kapodistrian University of Athens, Summer 1998.

45. "Spin-Orbit Splittings in Mg^{+}-Neutral Complexes", S. Matsika and R. M. Pitzer, The Fifth Sostrup Summer School: Quantum Chemistry and Molecular Properties, June 21- July 3, 1998, Aarhus, Denmark (poster).

46. "The Electronic Spectrum of the Neptunyl Ion, NpO_2^{2+}", S. Matsika and R. M. Pitzer, 53rd Ohio State University International Symposium on Molecular Spectroscopy, June 15-19, 1998; Paper RB04.

47. "Ab Initio Study of $MgAr^{+}$ and $MgXe^{+}$", S. Matsika and R. M. Pitzer, 52nd Ohio State University International Symposium on Molecular Spectroscopy, June 16-20, 1997; Paper RB02.

48. "Ab Initio Study of Weakly Bound Complexes of Mg Ion with Rare Gas Atoms", Department of Chemistry, The Ohio State University, May 30, 1997.

CURRENT FUNDING

National Science Foundation, "Quantum chemical methods for studying photon and electron driven processes in biological systems", 04/1/ 2023- 03/30/2026, Total : $533,698

Department of Energy, "Combining High Level Ab Initio Calculations with Laser Control of Molecular Dynamics", 02/15/2024 - 02/14/2027, Total : $500,000

PREVIOUS FUNDING

Department of Energy, "Computational Chemical Science Center: Chemistry in Solution and at Interfaces (CSI)" (co-PI), 09/15/2022 - 04/02/2025, Total : $1,729,056

National Science Foundation, "Collaborative Research: Understanding Ultrafast Observables", 06/1/ 2021- 05/30/2025, Total: $234,000

National Institute of Health, "MARC at Temple University", (contact PI), 06/01/2020 – 05/31/2025, Total: $2,058,292

Department of Energy, "Combining High Level Ab Initio Calculations with Laser Control of Molecular Dynamics", 11/15/2020 - 02/14/2024, Total : $465,000

National Science Foundation, "Quantum chemical methods for studying photon and electron driven processes in biological systems", 07/1/ 2018- 06/30/2022, Total : $533,698

Department of Energy, "Computational Chemical Science Center: Chemistry in Solution and at Interfaces (CSI)" (co-PI), 09/15/2018 - 09/14/2022, Total : $1,361,105

Department of Energy, "Combining High Level Ab Initio Calculations with Laser Control of Molecular Dynamics", 11/15/2017 - 11/14/2020, Total : $405,000

National Science Foundation, "Quantum chemical methods for studying photon and electron driven processes in biological systems", 05/1/ 2015- 04/30/2019, Total : $480,000

Department of Energy, "Combining High Level Ab Initio Calculations with Laser Control of Molecular Dynamics", 11/15/2014 - 11/14/2017, Total : $300,000

National Science Foundation, "Quantum chemical methods for studying photoinitiated processes in biological systems", 07/1/ 2012- 06/30/2015, Total : $411,000

Department of Energy, "Combining High Level Ab Initio Calculations with Laser Control of Molecular Dynamics", 02/15/2011 - 11/14/2014, Total : $300,000

National Science Foundation, "Theoretical Studies of Nonadiabatic Photoinitiated Processes in Complex Systems ", 08/01/ 2009- 07/31/2012, Total : $405,000

Department of Energy, "Combining High Level Ab Initio Calculations with Laser Control of Molecular Dynamics", 08/15/2008 - 02/14/2011, Total : $200,000 (Collaboration with Thomas Weinacht at SUNY, Stony Brook)

National Science Foundation, "CAREER: Theoretical Studies of Nonadiabatic Photoinitiated Processes in Complex Systems ", 01/01/ 2005- 12/30/2009, Total : $448,999

The ACS Petroleum Research Fund: PRF-SE "Excited Electronic States in Chemistry and Biology: Theory and Experiment, at the ACS National Meeting, August 2007, Boston, MA", $2,400

DAAD Research Visit Grant for Faculty, (declined)

Temple University Internationalization Grant, September 2013-June 2014

Return of Overhead Research Incentive Grant Program, $30,000, August 1, 2004 - July 30, 2005

Grant-in-Aid, $1,200, July 1, 2004 - June 30, 2005

STUDENTS AND POSTDOCTORAL FELLOWS:

Postdoctoral Fellows:

Dr. ZongRong Xu (2004-2007)
Dr. Akihiko Yoshikawa (2005)
Dr. Dimitri Laikov (2007) (Senior researcher, Moscow State University, RUSSIA)
Dr. Pascal Krause (2009-2012) (Gottfried Wilhelm Leibniz Universität Hannover: Hannover, DE)
Dr. Kurt A. Kistler (2010-2011) (Prof at Penn State Brandywine)
Dr. Mariana Assmann (2013-2015) (UCL, England)
Dr. Wook Lee (2014 -2016) (Assistant Prof at Kangwon National University, S. Korea)
Dr. Tolga Karsili (2016 -2018) (Associate Prof. at the University of Louisiana)
Dr. James Brown (2016 - 2017) (qBraid Co)
Dr. Patricia Vindel Zandbergen (2018 - 2019) (postdoc, New York University)
Dr. Cate Anstöter (2020-2021) (Christina Miller Research Fellow, University of Edinburgh)
Dr. Divya Tripathi (2023 -2024) (postdoc at TIFR, India)
Dr. Juan Carlos San Vicente Veliz (2024-present)

Graduate Students:

Dr. Kurt A. Kistler (2004-2010) (18 papers published; currently Prof at Penn State Brandywine; Awards: CST outstanding research award, Swern Research Fellowship, Francis Case Research Award, CST graduate student travel award, poster prize at Philadelphia ACS meeting)
Dr. Zhen Lu (2009-2015) (5 papers published; co-founder and CEO, RunPod)
Ranjeetha Suryavanshi (2008-2009) (Asst. Prof. at JBIET, India)
Dr. Vincent Spata (2011 - 2016) (7 papers published; Awards: Swern Research Fellowship, Dissertation Completion Award)
Congyi Zhou (2009-2012) (7 papers published)
Mark Fennimore (2014-2018) (5 papers published; Quaker Houghton Chemicals)

Dr. Pratip Chakraborty (2015-2020) (11 papers published; Senior Research Associate at the U of East Anglia))
Dr. Salsabil Abou-Hatab (2017-2022) (7 papers published; postdoc at Drexel U; Awards: First Summer Research Initiative Award, Swern Research Fellowship)
Dr. Mushir Thodika (2017-2022) (7 papers published; Postdoc at National Renewable Energy Laboratory; Awards: Francis Case Research Award)
Dr. Mohammed Sorour (2018 - 2024) (6 papers published; scientist at Syensqo, Awards: Swern Research Fellowship, Guy Allen Award)
Dr. Vaibhav Singh (2019-2024) (5 papers published; Swern Research Fellowship)
Dakshitha Abeygunewardane (2021-present) (2 paper published)
Maneesh Pyla (2022-present)(2 paper submitted)
Hind Hamoud Alrushud (2024- present)
Kanishka Yasuru MKV (2025 -present)

Undergraduate Students:

Ruth Elliott (2004-2005) (1 paper published, first author; Diamond Scholar)
Kandis Gilliard, PhD (2005-2006) (1 paper published; AMP summer research scholarship, currently WiSE Gabilan Assistant Professor of Civil and Environmental Engineering at U of Southern California)
Madiyha Muhammad (Summer 2007)
Benjamin Mejia (Summer 2007)
Elizabeth Mburu, MD (2007-2008) (1 paper published, first author; Awards: Clearfield and Fineman CST awards)
Nickolas Crawford (Summer 2009)
Christopher Kozak (2008-2010) (1 paper published, first author; Awards: Philadelphia Section ACS award, currenlty at Dow Chemical)
Parth Patel (Spring 2010)
JingXin Liang, PhD (2009-2012) (2 papers published, first author; Diamond Peer Teacher, Diamond Research scholar, Awards: Tomlison award, the Conwell Undergraduate Research Award, the Henry A. Sloviter Student Research Award in Chemistry, and a University Scholarship, NSF GRFP fellowship, PhD from Caltech)
Quynh Nguyen, PhD (2012-2014) (2 papers published, first author; NSF GRFP fellowship, PhD from U. Colorado Boulder, currently scientist at Stanford)
Catherine Triandafillou, PhD (2011-2013) (1 paper published, first author; American Institute of Chemists (AIC) Award, NSF GRFP fellowship) (PhD from University of Chicago, currently postdoc at UPenn)
Stephen Meloni, PhD (Summer 2012-Spring 2014) (1 paper published, first author; PhD from UPenn)
Thuylinh Cao (Fall 2013 - Spring 2014)
Dillion Fox, PhD (Spring 2014) (PhD from UPenn, currently at GSK)
Yang Zeng (Spring 2015)
Aya Matsumura (Spring 2015 -Summer 2015) (recipient of the Philadelphia Section ACS Award
Salsabil Abou-Hatab, PhD (Spring 2015-Spring 2016)(1 paper published, first author; PhD from Temple, currently postdoc at Drexel)
Margaret Anne King (Summer 2016)
Chey Jones, PhD (Fall 2014 - Spring 2017), (Awards: Philadelphia Section ACS award, NSF GRFP fellowship; PhD from Stanford University, currently at Merck)
Michael Bennett (Summer 2016 - Spring 2017)
Linh Nguyen (Summer 2017- Spring 2018) (1 paper published)
Abigail Serridge (Summer 2018)

Davielle Matos (Summer 2019, NSF-REU)
Drew Behrendt (Summer 2019-Spring 2020), (Awards: ACS Physical Chemistry; currently a PhD student at UPenn)
Camilo Zuluaga (Summer 2019-Summer 2020), (1 paper published, first author, currently a PhD student at Boston U)
Nathan MacKouse (Summer 2020 -Spring 2021), (1 paper published, Awards: ACS Physical Chemistry, currently at Merck)
Khai Nguyen (Summer 2020 -Spring 2021), (currently PhD student at Vanderbilt Institute of Imaging Science)
Griffin O'Neill (Summer 2021-Fall 2021)
Nicholas Baker (Summer 2021-Spring 2022) (currently at Tufts Medical School)
Christian Mobo (Summer 2022-Spring 2023) (Awards: ACS Physical Chemistry, currently TA at Temple U)
Jordan Howe (Spring 2022-Spring 2024), (1 paper published, first author, currently at Temple Professional Science Master's Bioinformatics)
Carson Baker (Fall 2022-Summer 2024), (Awards: ACS Physical Chemistry; currently PhD student at USC)
Sabrina Murodova (Spring 2023-Spring 2024)
Ryan Kulyassa (Summer 2024, NSF-REU)
Jose Mendez-Guerra (Fall 2023- May 2025)
Jay Ragbirsingh (Spring 2024-present)
Trevor Long (Summer 2025-present)
Alexander Espinoza (Summer 2025, NSF-REU)

High School Students:
Carina Tse (2015-2017)
Palak Shah (2017 - 2018)
Mazin Ahmed (2018)
Megan Chan (2023)
Jenny Nguyen (2023)
Nashia Nahid (2024, 2025)
Claudia Kim (2024)
Marlayna Lichtenstein(2025)
Christian Feil (Fall 2025)