

**CURRICULUM VITAE**  
**Spiridoula Matsika, Ph.D**

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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**

- 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
- Inter-American Photochemical Society

## TEACHING ACTIVITIES:

S 04	Chem 636: Molecular Spectroscopy
F 04, 05, 06, 08, 09, 16	Chem 5301: Quantum Chemistry
S 05, 07, 09, 12, 17, F 07, 14	Chem 3302 (old Chem 232): Physical Chemistry II
S 06	Chem 738: Special Topics in Phys. Chem: Computational Chemistry
S 08, 13, 15, F 17, F 18	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	Chem 3405: Physical Chemistry of Biomolecules

## SERVICE ACTIVITIES:

### *Professional:*

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, (Agencies: reviewed individual proposals and/or served on panels) NSF, PRF, DOE, AFOSR
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)
Workshop	
Leader:	CATALYST Conference: workshop for middle school girls, Swarthmore College, March 2012, 2015
Member:	Editorial Advisory Board of the Journal of Physical Chemistry, 2014-2016 Committee of Sciences and the Arts (CSA) of the Franklin Institute, 2014-present Editorial Committee of the Annual Review of Physical Chemistry, 2016- present 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-present
Co-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

*Collegial:*

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

*Departmental:*

2003-2005, 2007-2008	Presidential Faculty Search Committee
Summer 2004-2007	Graduate Recruiting Committee
Spring 2007-2016	Graduate Admissions Committee
Fall 2007-present	Undergraduate Curriculum Analysis and Development Committee
Fall 2014-2019	Chair, Undergraduate Curriculum Analysis and Development Committee
Fall 2009-present	Undergraduate Faculty Advisor

## **PUBLICATIONS**

(116 total (h index=28 (Web of Science)))

1. 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.*, submitted, 2020
2. 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) <https://doi.org/10.1063/5.0005558>
3. “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. Araújo 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)
4. “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) <https://doi.org/10.1063/1.5134700>
5. “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) DOI: 10.1103/PhysRevA.00.003400
6. “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) DOI: 10.1021/acs.jpcc.9b05961
7. “Intersystem crossing in the exit channel”, Hongwei Li, Alexander Kamasah, Spiridoula Matsika, Arthur G. Suits, *Nature Chemistry*, **11**, 123, (2019)

8. "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)
9. "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)
10. "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)
11. "The Origin of Fluorescence in DNA Thio-Analogues", Tolga N. V. Karsili, Mushir Thodika, Linh Nguyen, Spiridoula Matsika *Chem. Phys.*, **515**, 434-440, (2018)
12. "Introduction: Theoretical Modeling of Excited State Processes", Spiridoula Matsika and Anna I. Krylov, *Chem. Rev.*, **118**, 6925-6926, (2018)
13. "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)
14. "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)
15. "Electronic Resonances of Nucleobases Using Stabilization Methods", Mark A. Fennimore, and Spiridoula Matsika, *J. Phys. Chem. A*, **122**, 4048-4057, (2018)
16. "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)
17. "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)
18. "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)
19. "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)
20. "Vibrationally Assisted Below Threshold Ionization", Spencer L. Horton, Yusong Liu, Pratip Chakraborty, Spiridoula Matsika, and Thomas Weinacht, *Phys. Rev. A*, **95**, 063413, (2017)
21. "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)
22. "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)
23. "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)

24. "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)
25. "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)
26. "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)
27. "Photophysical Properties of Pyrrolocytosine, a Cytosine Fluorescent Base Analogue", Nguyen, Quynh, Vincent A. Spata, Spiridoula Matsika, *Phys.Chem.Chem.Phys.*, **18**, 20189-20198, (2016)
28. "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)
29. "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**, pp 3233 - 3240, (2016)
30. "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)
31. "Surface hopping investigation of the relaxation dynamics in radical cations", Mariana Assmann, Thomas Weinacht, and Spiridoula Matsika, *J. Chem. Phys.*, **144**, 034301 (2016)
32. "Photophysical Deactivation Pathways in Adenine Oligonucleotides", Vincent A. Spata and Spiridoula Matsika, *Phys.Chem.Chem.Phys.*, **17**, 31073 (2015)
33. "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)
34. "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)
35. "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)
36. "Photoelectron spectrum and dynamics of the uracil cation", Mariana Assmann, Horst Köppel and Spiridoula Matsika, *J. Phys. Chem. A*, **119**, 866-875, (2015)
37. "Modified Nucleobases", S. Matsika, "Topics in Current Chemistry - Photoinduced Phenomena in Nucleic Acids" (DOI:10.1007/128\_2014\_532), **355**, 209-243, (2015)
38. "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)
39. "Tribute to David R. Yarkony", Spiridoula Matsika, Henry F. Schaefer, III, and Michael S. Schuurman, *J. Phys. Chem. A*, **118**, 11837 - 11837, (2014)
40. "What We Can Learn from the Norms of One-particle Density Matrices, and What We Can't", Matsika, Spiridoula; Feng, Xintian; Luzanov, Anatoly; Krylov, Anna, *J. Phys. Chem. A* **118**, 11943-11955, (2014), (DOI: 10.1021/jp506090g)

41. "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), (DOI:10.1021/jp507520c)
42. "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)
43. "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)
44. "Ultrafast Excited-State Dynamics and Vibrational Cooling of 8-oxo-7,8-dihydro-2-deoxyguanosine in D<sub>2</sub>O", 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)
45. "Measurement of Ionic Resonances in Alkyl Phenyl Ketone Cations via Infrared Strong Field Mass Spectrometry", Bohinski, Tim; Moore Tibbetts, Katharine; Tarazkar, Maryam; Romanov, Dmitri; Matsika, Spiridoula; Levis, Robert, *J. Phys. Chem. A*, **117**, 12374 - 12381, (2013)
46. "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)
47. "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)
48. "Dissociative electron attachment to carbon dioxide via the <sup>2</sup>Π<sub>u</sub> 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)
49. "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)
50. "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)
51. "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")
52. "Measurement of an Electronic Resonance in Ground State, Gas Phase Acetophenone Cation via Strong Field Mass Spectrometry", T. Bohinski, K. M. Tibbetts, M. Tarazkar, D. Romanov, S. Matsika, R. J. Levis, *J. Phys. Chem. Lett.*, **4**, 1587 - 1591, (2013)
53. "Angle-Resolved Strong Field Ionization of Polyatomic Molecules: More than the Orbitals Matters", O. Njoya, S. Matsika and T. Weinacht, *ChemPhysChem*, **14**, 1451-1455, (2013)
54. "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)
55. "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)

56. "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)
57. "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)
58. "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)
59. "Fragmentation Pathways in the Uracil Radical Cation", C. Zhou, S. Matsika, M. Kotur and T. Weinacht, *J. Phys. Chem. A*, **116**, 9217-9227, (2012)
60. "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)
61. "On the Accessibility to Conical Intersections in Purines: Hypoxanthine and its Singly Protonated and Deprotonated Forms", J. Peon, J. Villabona-Monsalve, R. Noria and S. Matsika, *J. Am. Chem. Soc.*, **134**, 7820 - 7829, (2012)
62. "Two Dimensional Fourier-Transform Spectroscopy of Adenine and Uracil Using Shaped Ultrafast Laser Pulses in the Deep UV", C. Tseng, P. Sandor, M. Kotur, T. C. Weinacht and S. Matsika, *J. Phys. Chem. A*, **116**, 2654, (2012)
63. "High-multiplicity natural orbitals in multireference configuration interaction for excited states", Z. Lu and S. Matsika, *J. Chem. Theory Comput.*, **8**, 509-517, (2012)
64. "Nuclear Dynamics on a Three-state Jahn-Teller Model System", P. Krause and S. Matsika, *J. Chem. Phys.*, **136**, 034110 (2012)
65. "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)
66. "Following Ultrafast Radiationless Relaxation Dynamics With Strong Field Dissociative Ionization: A Comparison Between Adenine, Uracil, and Cytosine", M. Kotur, T. Weinacht, C. Zhou, and S. Matsika, *IEEE Journal of selected topics in Quantum Electronics*, **18**, 187-194, (2012)
67. "Strong Field Molecular Ionization from Multiple Orbitals", M. Kotur, T. Weinacht, C. Zhou and S. Matsika, *Phys. Rev. X*, **1**, 021010, (2011)
68. "Combining dissociative ionization pump probe spectroscopy and ab initio calculations to explore excited state dynamics involving conical intersections", S. Matsika, C. Zhou, M. Kotur and T. Weinacht, *Faraday Discussions*, **153**, 247 - 260, (2011)
69. "Distinguishing Between Relaxation Pathways by Combining Dissociative Ionization Pump Probe Spectroscopy and ab initio Calculations: A Case Study of Cytosine ", M. Kotur, T. Weinacht, C. Zhou, K. A. Kistler, and S. Matsika, *J. Chem. Phys.*, **134**, 184309, (2011)
70. "Pathways for fluorescence quenching in 2-aminopurine  $\pi$ -stacked with pyrimidine nucleobases", J.X. Liang and S. Matsika, *J. Am. Chem. Soc.*, **133**, 6799 - 6808, (2011); Correction: *J. Am. Chem. Soc.*, **134**, 10713 - 10714, (2012)
71. "Nonadiabatic Events and Conical Intersections", S. Matsika and P. Krause, *Annu. Rev. Phys. Chem.*, **62**, 621 - 643, (2011)
72. "Three-state conical intersections", S. Matsika, Chapter in "Conical Intersections: Theory, Computation and Experiment", *Advanced Series in Physical Chemistry - Vol. 17*, 83-116, World Scientific Publishing Company, February 2011

73. "Photophysical Pathways of Cytosine in Aqueous Solution", K. A. Kistler and S. Matsika, *Phys. Chem. Chem. Phys.*, **12**, 5024 - 5031, (2010)
74. "Excited State Energies and Electronic Couplings of DNA Base Dimers", C. R. Kozak, K. A. Kistler, Z. Lu and S. Matsika, *J. Phys. Chem. B*, **114**, 1674-1683, (2010)
75. "Change in Electronic Structure upon Optical Excitation of 8-Vinyladenosine: An Experimental and Theoretical Study", G. Kodali, K. A. Kistler, M. Narayanan, S. Matsika and R. Stanley, *J. Phys. Chem. A*, **114**, 256 - 267, (2010)
76. "Solvatochromic Shifts of Uracil and Cytosine Using a Combined Multireference Configuration Interaction/ Molecular Dynamics Approach and the Fragment Molecular Orbital Method", K. A. Kistler and S. Matsika, *J. Phys. Chem. A*, **113**, 12396-12403, (2009)
77. "Two-Dimensional Ultrafast Fourier Transform Spectroscopy in the Deep Ultraviolet", C. Tseng, S. Matsika, T. Weinacht, *Optics Express*, **17**, 18788-18793, (2009)
78. "Closed-Loop Learning Control of Isomerization using Shaped Ultrafast Laser Pulses in the Deep Ultraviolet", M. Kotur, T. Weinacht, B. J. Pearson and S. Matsika *J. Chem. Phys.*, **130**, 134311, (2009)
79. "State-resolved distribution of OH X<sup>2</sup>Π products arising from electronic quenching of OH A<sup>2</sup>Σ<sup>+</sup> by N<sub>2</sub>", L. P. Dempsey, T. D. Sechler, C. Murray, M. Lester, and S. Matsika *J. Chem. Phys.*, **130**, 104307, (2009)
80. "Quantum Mechanical Studies of the Photophysics of DNA and RNA bases", K. A. Kistler and S. Matsika, a chapter for "Multi-scale Quantum Models for Biocatalysis: Modern Techniques and Applications" in the series CHALLENGES AND ADVANCES IN COMPUTATIONAL CHEMISTRY AND PHYSICS, guest eds. Tai-Sung Lee and Darrin M. York, series editor Jerzy Leszczynski, Vol. 7, Chapter 11, p. 285, (2009)
81. "An Ab Initio Study of Substituent Effects on the Excited States of Purine Derivatives", E. Mburu and S. Matsika, *J. Phys. Chem. A*, **112**, 12485 - 12491, (2008)
82. "On the Electronically Excited States of Uracil", E. Epifanovsky, K. Kowalski, P.-D. Fang, M. Valiev, S. Matsika, A. I. Krylov, *J. Phys. Chem. A*, **112**, 9983 - 9992, (2008)
83. "Three-State Conical Intersections in Cytosine and Pyrimidinone Bases", K. A. Kistler and S. Matsika, *J. Chem. Phys.*, **128**, 215102, (2008)
84. "Two- and Three-State Conical Intersections in Uracil Cation Radical", S. Matsika, *Chem. Phys.*, **349**, 356-362, (2008) (invited article for the special issue in honor of H. Lischka)
85. "Interpreting Ultrafast Molecular Fragmentation Dynamics with *Ab Initio* Calculations", C. Trallero, B. J. Pearson, T. Weinacht, K. Gilliard and S. Matsika, *J. Chem. Phys.*, **128**, 124107, (2008)
86. "2-Aminopurine Excited State Electronic Structure Measure by Stark Spectroscopy", G. Kodali, K. A. Kistler, S. Matsika and R. J. Stanley, *J. Phys. Chem. B*, **112**, 1789-1795, (2008)
87. "Excited Electronic States and Photophysics of Uracil-Water Complexes", A. Yoshikawa and S. Matsika, *Chem. Phys.*, **347**, 393-404, (2008) (invited article for the special issue in honor of W. Domcke)
88. "Inclusion of Second-order Correlation Effects for the Ground and Singly Excited States Suitable for the Study of Conical Intersections: The CIS(2) Model", *Chem. Phys. Lett.*, D. Laikov and S. Matsika, **448**, 132-137, (2007)
89. "Cytosine in Context: A Theoretical Study of Substituent Effects on the Excitation Energies of 2-Pyrimidinone Derivatives", K. A. Kistler and S. Matsika, *J. Phys. Chem. A*, **111**, 8708-8716, (2007)

90. "6MAP, a fluorescent adenine analogue, is a probe of base flipping by DNA photolyase", K. Yang, S. Matsika and R. J. Stanley, *J. Phys. Chem. B*, **111**, 10615-10625, (2007)
91. "Radiationless Decay Mechanism of Cytosine: An Ab Initio Study with Comparisons to the Fluorescent Analogue 5-Methyl-2-Pyrimidinone", K. A. Kistler and S. Matsika, *J. Phys. Chem. A*, **111**, 2650-2661, (2007)
92. "The Fluorescence Mechanism of 5-Methyl-2-Pyrimidinone: An *Ab Initio* Study of a Fluorescent Pyrimidine Analog", K. A. Kistler and S. Matsika, *Photochemistry and Photobiology*, **83**, 611-624, (2007) (invited article for the special issue on DNA Excited States)
93. "Conical intersections in Molecular Systems", S. Matsika, *Rev. Comp. Chem.*, Vol. **23**, p. 83, (2007) (invited review)
94. "A Combined Multireference Configuration Interaction/Molecular Dynamics Approach for Calculating Solvatochromic Shifts: Application to the  $n_O \rightarrow \pi^*$  Electronic Transition in Formaldehyde", Z. Xu and S. Matsika, *J. Phys. Chem. A*, **110**, 12035-12043, (2006)
95. "Excited Electronic States of the Cyclic Isomers of O<sub>3</sub> and SO<sub>2</sub>", R. Elliot, R. Compton, R. J. Levis, and S. Matsika, *J. Phys. Chem. A*, **109**, 11304 - 11311, (2005)
96. "Three-State Conical Intersections in Nucleic Acid Bases", S. Matsika, *J. Phys. Chem. A*, **109**, 7538 - 7545, (2005)
97. "Radiationless Decay of Excited States of Uracil through Conical Intersections", S. Matsika, *J. Phys. Chem. A*, **108**, 7584-7590, (2004)
98. "Quantitative Detection of Singlet O<sub>2</sub> via Cavity Enhanced Absorption", S. Williams, M. Gupta, T. Owano, D. S. Baer, A. O'Keefe, D. R. Yarkony and S. Matsika, *Optics Letters*, **29**, 1066-1068, (2004)
99. "Conical Intersections of Three Electronic States Affect the Ground State of Radical Species with Little or No Symmetry: Pyrazolyl", S. Matsika and D. R. Yarkony, *J. Am. Chem. Soc.*, **125**, 12428-12429, (2003)
100. "Beyond Two-State Conical Intersections. Three-State Conical Intersections in Low Symmetry Molecules: the Allyl Radical ", S. Matsika and D. R. Yarkony, *J. Am. Chem. Soc.*, **125**, 10672-10676, (2003)
101. "Photodissociation of the Vinyloxy Radical through Conical, and Avoided, Intersections", S. Matsika and D. R. Yarkony, *J. Chem. Phys.*, **117**, 7198-7206, (2002)
102. "Accidental Conical Intersections of Three States of the Same Symmetry. I. Location and Relevance", S. Matsika and D. R. Yarkony, *J. Chem. Phys.*, **117**, 6907-6910, (2002)
103. "Spin-Orbit Coupling and Conical Intersections . IV. A Perturbative Determination of the Electronic Energies, Derivative Couplings and a Rigorous Diabatic Representation near a Conical Intersection. The General Case", S. Matsika and D. R. Yarkony, *J. Phys. Chem. B*, **106**, 8108-8116, (2002)
104. "Conical Intersections and the Nonadiabatic Reactions  $H_2O+O(^3P) \leftrightarrow OH(A^2\Sigma^+)+OH(X^2\Pi)$ ", S. Matsika and D. R. Yarkony, *J. Chem. Phys.*, **117**, 3733-3740, (2002)
105. "Conical Intersections and the Spin-Orbit Interaction", S. Matsika and D. R. Yarkony, *The Role of Degenerate States in Chemistry: A Special Volume of Advances in Chemical Physics*, **124**, 557-581, (2002)
106. "Intersecting Conical Intersection Seams: their Location, Representation, and Effect on Local Topography", S. Matsika and D. R. Yarkony, *J. Phys. Chem. A*, **106**, 2580-2591, (2002)

107. "Spin-Orbit Coupling and Conical Intersections in Molecules with an Odd Number of Electrons. III. A Perturbative Determination of the Electronic Energies, Derivative Couplings and a Rigorous Diabatic Representation near a Conical Intersection", S. Matsika and D. R. Yarkony, *J. Chem. Phys.*, **116**, 2825-2835, (2002)
108. "On the Effects of Spin-Orbit Coupling on Conical Intersection Seams in Molecules with an Odd Number of Electrons. II. Characterizing the Local Topography of the Seam", S. Matsika and D. R. Yarkony, *J. Chem. Phys.*, **115**, 5066-5075, (2001)
109. "On the Effects of Spin-Orbit Coupling on Conical Intersection Seams in Molecules with an Odd Number of Electrons. I. Locating the Seam", S. Matsika and D. R. Yarkony, *J. Chem. Phys.*, **115**, 2038-2050, (2001)
110. "Electronic Structure and Spectra of Actinyl Ions", S. Matsika, Z. Zhang, S. R. Brozell, J.-P. Blaudeau, Q. Wang, and R. M. Pitzer, *J. Phys. Chem. A*, **105**, 3825-3828, (2001)
111. "Actinyl Ions in  $\text{Cs}_2\text{UO}_2\text{Cl}_4$ ", S. Matsika and R. M. Pitzer, *J. Phys. Chem. A*, **105**, 637-645, (2001)
112. "Intensities in the Spectra of Actinyl Ions", S. Matsika, R. M. Pitzer and D. T. Reed, *J. Phys. Chem. A*, **104**, 11983-11992, (2000)
113. "The Electronic Spectrum of the  $\text{NpO}_2^{2+}$  and  $\text{NpO}_2^+$  Ions", S. Matsika and R. M. Pitzer, *J. Phys. Chem. A*, **104**, 4064-4068, (2000)
114. "Atomic Orbital Basis Sets for Use with Effective Core Potentials", J.-P. Blaudeau, S. R. Brozell, S. Matsika, Z. Zhang and R. M. Pitzer, *Int. J. Quantum Chem.*, **77**, 516-520, (2000)
115. "Spin-Orbit Splittings in  $\text{Mg}^+$ -Neutral Complexes", S. Matsika and R. M. Pitzer, *J. Phys. Chem. A*, **102**, 1652-1656, (1998)
116. "Ab Initio Study of the Ground and Several Excited States of the NLi System", S. Matsika, A. Papakonidylis and A. Mavridis, *Chem. Phys. Lett.*, **250**, 409-414, (1996)

#### INVITED TALKS AT CONFERENCES AND WORKSHOPS (75 total)

1. "Unraveling excited state dynamics and spectroscopy in organic chromophores", 2020 Pacific Conference on Spectroscopy and Dynamics, San Diego CA, Jan 30-Feb 2, 2020
2. "Using computers, physics and mathematics to understand chemistry and biology", APS Conference for Undergraduate Women in Physics, January 2020, Temple University
3. "Theoretical approaches to calculating resonances", Telluride workshop on "Advances in Theory of Electronic Resonances", July 22-26, 2019
4. "Nonadiabatic dynamics in photon and electron driven processes", Telluride workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", July 16-20, 2019
5. "Exploring Excited State Potential Energy Surfaces for Photon and Electron Driven Processes", Dynamics of Molecular Collisions, Montana, July 7-12, 2019
6. "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
7. "Modeling Photophysics and Photochemistry in Complex Systems", "Chemistry and Physics of Advanced Materials - III" symposium at IISER Pune, India, October 2018
8. "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

9. "Theoretical description of nonadiabatic events in photon and electron driven processes", 256th ACS National Meeting in Boston, MA, August 19-23, 2018
10. "Nonadiabatic events in photon and electron driven processes", Telluride Workshop on "Spectroscopy and Dynamics on Multiple Surfaces", Telluride, CO, July 2018
11. "Nonadiabatic Effects in Photon and Electron Driven Reactions", Molecular Interactions and Dynamics Gordon Research Conference, Easton, MA, July 8-13, 2018
12. "Theoretical studies of photochemistry in nucleic acids", ASP 2018 Biennial Meeting, Tampa, FL, 12-15 May 2018
13. "Nonadiabatic Dynamics in Condensed Phases", Gordon Conference on Molecular and Ionic Clusters, February 25- March 2, 2018, Italy
14. "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
15. "Theoretical insight into the photophysics and photochemistry related to DNA damage and repair", 13th Femtochemistry conference, Cancun, Mexico, August 12-17, 2017
16. "Interaction of nucleobases with low energy electrons", Telluride workshop on "Photo Physics of Biomolecular Ions", July 24-28, 2017
17. "Photophysics and photochemistry in oligonucleotides", Telluride workshop on "Photo Physics of Biomolecular Ions", July 24-28, 2017
18. "Resonances and Dissociative Electron Attachment in Uracil using Stabilization Methods", Telluride workshop on "Advances in theory of electronic resonances", July 17-21, 2017
19. "Insights into the nonadiabatic dynamics of radical cations", APS March Meeting, New Orleans, March 13-17, 2017
20. "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
21. "QM/MM Studies of Photoinitiated Processes in Complex Systems", New York Theoretical and Computational Chemistry Conference, NYU, Dec. 2, 2016.
22. "QM/MM Studies of Photoinitiated Processes in Complex Systems", Penn Conference on Theoretical Chemistry, August 2016.
23. "QM/MM Studies of Photoinitiated Processes in Complex Systems", ISTCP (International Symposium of Theoretical Chemical Physics), North Dakota, July 2016
24. "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
25. "QM/MM studies of excited states in complex systems", Pacificchem, Honolulu, HI, December 2015
26. "Obtaining insights into the dynamics of radical cations produced via strong field ionization", Pacificchem, Honolulu, HI, December 2015
27. "Combining High Level Ab Initio Calculations with Laser Control of Molecular Dynamics", AMOS DOE meeting, October 2015
28. "Nonadiabatic events in photoinitiated processes in molecules", Dynamics of Molecular Collisions, Asilomar, CA, July 2015
29. "Nonadiabatic Dynamics in the Photophysics and Photochemistry of DNA", 98th Canadian Chemistry Conference and Exhibition, Ottawa, Canada, June 2015
30. "Insights into the role of excimers/exciplexes in the photophysics and photochemistry of DNA", 249th American Chemical Society meeting in Denver, CO, March 2015

31. "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
32. "Exciplexes and conical intersections in  $\pi$ -stacked bases in DNA", Workshop on "Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", Telluride, CO, July 2013
33. Introduction to the Non-adiabatic Dynamics Session, Dynamics of Molecular Collisions, Granlibaken CA, July 2013
34. "Exciplexes and Conical Intersections in  $\pi$ -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
35. "Exploring nonadiabatic events with strong field molecular ionization", Gordon Research Conference on Molecular Energy Transfer, Vendura, CA, January 2013
36. "Nuclear Dynamics of Model Systems with Two and Three-State Conical Intersections", XXIst International Symposium on the Jahn-Teller Effect, Tsukuba, Japan, August 2012
37. "Theoretical developments for modeling excited states and conical intersections", 244th American Chemical Society meeting in Philadelphia, PA, August 2012
38. "Introduction to the Excited State Dynamics session", Gordon Research Conference on Electronic Spectroscopy and Dynamics, Bates College, Maine, July 2012
39. "Non-adiabatic events in interacting chromophores", Gordon Research Conference on Atomic and Molecular Interactions, Stonehill College, Easton, MA, July 2012
40. "Theoretical developments for studying excited states and their potential energy surfaces", Telluride Workshop on "Spectroscopy and Dynamics on Multiple Surfaces", July 2012
41. "UV radiation and the building blocks of DNA/RNA: What theoretical studies can tell us", Astrobiology Science Conference 2012, April 2012, Atlanta, GA
42. "Theoretical studies of photophysical events in  $\pi$ -stacked dimers of nucleobases", 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), September 2-8, 2011, Tokyo, Japan
43. "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
44. "Nonadiabatic events in  $\pi$ -stacked interacting chromophores", Telluride workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", July 5-8, 2011, Telluride, CO
45. "Theoretical studies of photophysical properties in  $\pi$ -stacked nucleobase dimers", 51st Sanibel Symposium, February 25 - March 1, 2011, St. Simons Island, Georgia
46. "Combining high level ab initio calculations with laser control of molecular dynamics", Pacificchem, December 15-20, 2010, Honolulu, Hawaii
47. "Theoretical studies of excited electronic states of nucleobase dimers", Pacificchem, December 15-20, 2010, Honolulu, Hawaii
48. "Theoretical developments for modeling excited states and nonadiabatic effects", Pacificchem, December 15-20, 2010, Honolulu, Hawaii
49. "Conical intersections in non-isolated chromophores", XX International Symposium on the Jahn-Teller Effect, 16th - 20th August 2010, University of Fribourg, Switzerland
50. "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
51. "Excited electronic states of nucleobase dimers", 239th ACS National Meeting, March 21-25, 2010, San Francisco, CA

52. "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
53. "Excited states and conical intersections in non-isolated chromophores", 238th National ACS Meeting, Washington DC, August 2009
54. "The role of conical intersections in the photophysics of biologically relevant molecules", Gordon Conference on Electronic Spectroscopy and Dynamics, Colby College, Maine, July 2009
55. "Two- and three-state conical intersections in molecular systems", Department of Energy, Basic Energy Sciences, Combustion (Gas Phase Chemical Physics), May 2009
56. "Non-adiabatic Effects on Excited States of Biomolecules", 237th National ACS Meeting, March 22-26, 2009, Salt Lake City, Utah
57. "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
58. "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
59. "Couplings of excited states within and between nucleic acid bases". Telluride Workshop on "Spectroscopy and Dynamics on Multiple Surfaces", July 2008
60. "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
61. "Exploring two- and three-state conical intersections between electronic states of molecular systems", 48th Sanibel Symposium, February 2008
62. "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
63. "Photophysics of DNA/RNA Bases and their Analogs", 2007 MARM Meeting, Ursinus College, Collegeville, PA, May 17, 2007
64. "Electronically Excited States and Conical Intersections in Cytosine and its Analogs", 2007 APS March Meeting, Denver, CO, March 5-9, 2007
65. "Substituent Effects on the Excited Electronic States of Cytosine Analogs", 54th annual Western Spectroscopy Association Conference, Asilomar, CA, January 31-February 2, 2007.
66. "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
67. 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
68. "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
69. "Photophysical Properties of Pyrimidine Bases", 17th Inter-American Photochemical Society Conference, Salvador, Bahia, Brazil, June 2006
70. "Determination of Electronically Excited States and Conical Intersections by High Level Ab Initio Methods", 21<sup>th</sup> Austin Symposium on Molecular Structure, March 2006

71. "Role of Two- and Three-State Conical Intersections in the Photophysics of DNA and RNA Bases", Pacificchem, Honolulu, Hawaii, December 2005
72. "Two- and Three-State Conical Intersections in Complex Systems" 230th ACS National Meeting, August 2005, Washington, DC; Paper PHYS 181.
73. "A Hybrid QM/MM Approach Using Ab Initio MRCI Wavefunctions" workshop on COLUMBUS, Argonne National Laboratory, Chicago, IL, August 2005
74. "Two-state and Three-state Conical Intersections Affecting the Spectroscopy and Dynamics of Radicals", Telluride workshop on Dynamics of Atmospheric Radicals, Telluride; July 2004
75. "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 (58 total)**

1. "Using Hermitian and Non Hermitian Quantum Mechanics to Understand Molecular Reactivity", Department of Mathematics, Temple University, January 2020
2. "Modeling Photophysics and Photochemistry in Complex Systems", TIFR, India, October 2018
3. "Modeling Photochemistry and Electron Driven Chemistry", Texas A&M, September 25, 2018
4. "Modeling photophysics and photochemistry related to DNA damage", Villanova University, March 23, 2018
5. "Nonadiabatic events in photoinitiated processes in molecules", Stony Brook University, March 23, 2017
6. "Modeling Photophysics and Photochemistry in Biological Molecules", University of Southern California, Los Angeles, CA, February 13, 2017
7. "Modeling Photophysics and Photochemistry in Biological Molecules", UC Boulder, CO, November 11, 2016
8. "Modeling photoinitiated processes related to DNA damage", Bowling Green State University, February 24, 2016
9. "Photophysics and photochemistry related to DNA damage", University of Kansas, October 16, 2015
10. "Photoinitiated processes in biologically relevant molecules", Department of Physics, Temple University, September 14, 2015
11. "Modeling Photophysics and Photochemistry in Biological Molecules", Johns Hopkins University, April 7, 2015
12. "Investigating photoinduced processes in biologically relevant molecules", Wayne State University, November 12, 2014
13. "Exploring nonadiabatic events in photoinitiated processes in molecules", Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, June 20, 2014
14. "Photoinitiated processes in biologically relevant molecules", Iowa State University, January 31, 2014
15. "Using quantum chemistry and strong field dissociative ionization pump-probe spectroscopy to investigate photoinitiated processes in molecules", University of Vienna, December 17, 2013
16. "Using quantum chemistry and strong field dissociative ionization pump-probe spectroscopy to investigate photoinitiated processes in molecules", Technical University of Munich, December 5, 2013
17. "Mechanistical insights into fluorescence properties of DNA chromophores and fluorescent analogs", University of Siena, November 20, 2013

18. “Mechanistical insights into fluorescence properties of DNA chromophores and fluorescent analogs”, ICCOM U.O.S. di Pisa, November 19, 2013
19. “Mechanistical insights into fluorescence properties of DNA chromophores and fluorescent analogs”, Ludwig Maximilians- University of Munich, November 13, 2013
20. “Using quantum chemistry and strong field dissociative ionization pump-probe spectroscopy to investigate photoinitiated processes in molecules”, Karlsruhe Institute of Technology, November 11, 2013
21. “Investigating photoinitiated processes in biologically relevant molecules”, University of Heidelberg, Heidelberg, Germany, October 7, 2013
22. “How Quantum Mechanics explains the photostability of DNA under UV radiation”, National and Kapodistrian University of Athens, Greece, May 20, 2013
23. “How Quantum Mechanics explains the photostability of DNA under UV radiation”, University of Ioannina, Greece, May 28, 2013
24. “Theoretical studies of photoinitiated processes in biologically relevant molecules”, University of Wisconsin-Madison, April 15, 2013
25. “Quantum chemical studies of photoinitiated events in biological molecules”, Löwdin Lectures 2012, Uppsala University, November 23, 2012
26. “What molecules do when they get excited”, Löwdin Lectures 2012, Uppsala University, November 22, 2012
27. “Modeling photophysics and photochemistry in biological molecules”, University of Louisville, October 19, 2012
28. “Photophysical properties of biologically relevant molecules: A theoretical look”, Drexel University, March 8, 2012
29. “The role of conical intersections in photoinitiated processes of biologically relevant molecules”, University of California, Davis, January 24, 2012
30. “The role of conical intersections in photoinitiated processes of biologically relevant molecules”, Lawrence Berkeley National Laboratory, January 23, 2012
31. “ Modeling photoinitiated processes in DNA”, Institute for Molecular Science, Okazaki, Japan, September 9, 2011
32. “Conical Intersections in Photoinitiated Processes”, CST 10th Anniversary Celebration, Temple University, November 19, 2008
33. “The role of conical intersections in the photophysics of DNA/RNA bases and their analogs”, seminar at the University of Pennsylvania, October 2, 2008
34. “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
35. “Theoretical insight into the interaction of light with DNA”, seminar at Widener University, March 2008
36. “Photophysics of natural nucleobases and their analogs: turning the fluorescence on”, seminar at the University of Minnesota, MN, November 7, 2007
37. “Theoretical aspects of the photophysical behavior of natural nucleobases and their analogs”, seminar at The Ohio State University, Columbus, OH, November 5, 2007

38. "Photophysical Behavior and Photostability in DNA and RNA bases", seminar at Bryn Mawr, Philadelphia, PA, March 2, 2007.
39. "Photophysical Behavior and Photostability in DNA and RNA bases", seminar at the University of the Sciences in Philadelphia, Philadelphia, PA, January 29, 2007.
40. "Photophysical Behavior and Photostability in DNA and RNA bases" seminar at Florida International University, Miami, Florida, October 2006
41. "Nonadiabatic Photoinitiated Processes through Potential Energy Surface Crossings", seminar at SUNY at Stony Brook, April 2006
42. "Conical Intersections in Photochemistry and Photophysics", seminar at Los Alamos National Laboratory, Los Alamos, NM, October 2005
43. "Understanding Photoinitiated Processes through Potential Energy Surface Crossings" seminar at University of Southern California, Los Angeles, CA, October 2005
44. "Solving the Schrödinger Equation to Understand the Photostability of Biomolecules" seminar at the Department of Mathematics, Temple University, Philadelphia; April 2005
45. "Nonadiabatic Photoinitiated Processes and Photostability in Nucleobases", seminar at Johns Hopkins University, Maryland; February 2005
46. "Photoinitiated Processes in Chemistry and Biology: What do Potential Energy Surface Crossings Tell us about them", seminar at Shippensburg University, Pennsylvania; October 2004
47. "What do Conical Intersections have to do with Chemistry" seminar at the Department of Mathematics, Temple University, Philadelphia; March 2004
48. "Degenerate States in Chemistry", seminar at the Department of Physics, Temple University, Philadelphia; February 2004
49. "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
50. "Conical Intersections: Understanding Nonadiabatic Reactions in the Atmosphere, Photodissociation of Radicals, and Beyond", University of Memphis, Memphis, Tennessee, December 2002
51. "Conical Intersections: Understanding Nonadiabatic Reactions in the Atmosphere, Photodissociation of Radicals, and Beyond", Tulane University, Louisiana, December 2002
52. "Conical Intersections: Understanding Nonadiabatic Reactions in the Atmosphere, Photodissociation of Radicals, and Beyond", Florida State University, Tallahassee, Florida, November 2002
53. "Conical Intersections in Nonadiabatic Processes", National Institute of Standards and Technology, Gaithersburg, USA; February 2002.
54. "The Role of Conical Intersections in Nonadiabatic Processes", Washington University in St. Louis, St. Louis, USA; January 2002.
55. "Conical Intersections in Nonadiabatic Processes", Indiana University, Bloomington, Indiana, USA; January 2002.
56. "Actinyl Ions and the Effect of Ligands on Their Spectra", seminar at University of Bonn, Bonn, Germany; April 2001.
57. "Actinyl Ions and the Effect of Ligands on Their Spectra: the 5-Fold Way", seminar at Univ. Autonoma Madrid, Madrid, Spain; June 2000.

58. "Actinyl Ions and the Effect of Ligands on Their Spectra: the 5-Fold Way", seminar at Universite P. Sabatier, Toulouse, France; June 2000.

#### CONTRIBUTED PRESENTATIONS (44 total)

1. "Shape and Feshbach resonances of uracil", 252th American Chemical Society meeting, Philadelphia, PA, August 2016
2. "Dynamics on radical cations governed by conical intersections", March meeting of the American Physical Society, San Antonio, TX, March 2015
3. "Dynamics on radical cations governed by conical intersections", XXII International Symposium on the Jahn-Teller Effect, Austria, August 2014
4. "Bonded Excimer Formation in  $\pi$ -Stacked 9-Methyladenine Dimers", Gordon Research Conference on Photochemistry, Stonehill College, Easton, MA, July 2013 (poster presented by Vincent Spata)
5. "Get excited with High-Multiplicity Natural Orbitals", 244th American Chemical Society meeting, Philadelphia, PA, August 2012, (poster presented by Zhen Lu)
6. "Conical intersections in  $\pi$ -stacked nucleobase dimers containing 2-aminopurine", 244th American Chemical Society meeting, Philadelphia, PA, August 2012, (poster presented by JingXin Liang)
7. "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)
8. "Non-adiabatic events in  $\pi$ -stacked chromophores", Gordon Research Conference on Electronic Spectroscopy and Dynamics, Bates College, Maine, July 2012 (poster)
9. "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)
10. "Excited state coupling of adjacent thymine nucleobases", 237th American Chemical Society meeting, Salt Lake City, 2009, (poster presented by Christopher Kozak)
11. "Three-state conical intersections in cytosine and pyrimidinone bases", 237th American Chemical Society meeting, Salt Lake City, 2009, (presented by Kurt Kistler)
12. "Excited States of Non-isolated Chromophores", 64rd OSU International Symposium on Molecular Spectroscopy, Columbus, OH, June 2009
13. "Three-State Conical Intersections in Biologically Relevant Molecules", 64rd OSU International Symposium on Molecular Spectroscopy, Columbus, OH, June 2009
14. "Three-State Conical Intersections and their Signatures", American Conference on Theoretical Chemistry, Northwestern University, Evanston, IL, July 19-24, 2008 (poster)
15. "Three-state conical intersections in cytosine", 236th American Chemical Society meeting, Philadelphia, 2008, (poster presented by Kurt Kistler)
16. "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
17. "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)

18. "Two- and Three-State Conical Intersections Involved in the Photophysical Properties of Pyrimidine Molecules", 232th ACS National Meeting; San Francisco, CA, September 2006
19. "Two- and Three-State Conical Intersections in Complex Systems", APS meeting; Baltimore, MD, March 2006
20. "Photoinitiated processes in chemistry and biology: What do potential energy surface crossings tell us about them", Muhlenberg College, Allentown, PA; October 2005
21. "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)
22. "Radiationless Decay of Excited States in Nucleobases through Conical Intersections", 228th ACS National Meeting, August, 2004, Philadelphia, PA; Paper PHYS 500.
23. "Radiationless Decay of Excited States of Uracil through Conical Intersections", Gordon Research Conference on Atomic and Molecular Interactions, New London, NH, July 2004
24. "Beyond the Two-state Conical Intersections: Three-State Conical Intersections in Radicals ", 226th ACS National Meeting, September 2003, New York, NY; Paper COMP 85.
25. "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)
26. "Photodissociation of the Vinyloxy Radical through Conical Intersections and Avoided Crossings", S. Matsika and D. R. Yarkony, American Conference on Theoretical Chemistry; Champion, Pennsylvania; July 2002 (poster).
27. "Photodissociation of the Vinyloxy Radical through Conical Intersections and Avoided Crossings", S. Matsika and D. R. Yarkony, Gordon Conference: Atomic and Molecular Interactions; Rhode Island; July 2002 (poster).
28. "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).
29. "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.
30. "Intensities of the Electronic Spectrum of  $\text{NpO}_2^+$ ", S. Matsika and R. M. Pitzer, 55th Ohio State University International Symposium on Molecular Spectroscopy, June , 2000; Paper RH10.
31. "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.
32. "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.
33. "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.

34. "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.
35. "Actinyl ions in Cs<sub>2</sub>UO<sub>2</sub>Cl<sub>4</sub> Crystal", S. Matsika and R. M. Pitzer, 54th Ohio State University International Symposium on Molecular Spectroscopy, June 14-18, 1999; Paper RH11.
36. "Ab Initio Calculations of the Neptunyl Ion, NpO<sub>2</sub><sup>2+</sup>, and of the Dioxoneptunium(+1) Ion, NpO<sub>2</sub><sup>+</sup>", S. Matsika and R. M. Pitzer, Relativistic Effects in Heavy-Element Chemistry and Physics, 10-15 April, 1999, Acquafredda di Maratea, Italy; Poster P37.
37. "Ab Initio Calculations of the Neptunyl Ion, NpO<sub>2</sub><sup>2+</sup>, and of the Dioxoneptunium(+1) Ion, NpO<sub>2</sub><sup>+</sup>. 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.
38. "The Electronic Spectrum of the Neptunyl Ion, NpO<sub>2</sub><sup>2+</sup> and of NpO<sub>2</sub><sup>+</sup>", Computational Chemistry for Nuclear Waste Characterization and Processing: Relativistic Quantum Chemistry of Actinides, Workshop III at Lawrence Berkeley National Lab, September 17-19, 1998.
39. "The Electronic Spectrum of the Neptunyl Ion, NpO<sub>2</sub><sup>2+</sup>", Computational Chemistry for Nuclear Waste Characterization and Processing: Relativistic Quantum Chemistry of Actinides, Workshop II at Argonne National Lab, January 17-19, 1998.
40. "The Electronic Spectrum of the Neptunyl Ion, NpO<sub>2</sub><sup>2+</sup> and of NpO<sub>2</sub><sup>+</sup>", The National and Kapodistrian University of Athens, Summer 1998.
41. "Spin-Orbit Splittings in Mg<sup>+</sup>-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).
42. "The Electronic Spectrum of the Neptunyl Ion, NpO<sub>2</sub><sup>2+</sup>", S. Matsika and R. M. Pitzer, 53rd Ohio State University International Symposium on Molecular Spectroscopy, June 15-19, 1998; Paper RB04.
43. "Ab Initio Study of MgAr<sup>+</sup> and MgXe<sup>+</sup>", S. Matsika and R. M. Pitzer, 52nd Ohio State University International Symposium on Molecular Spectroscopy, June 16-20, 1997; Paper RB02.
44. "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", 07/1/ 2018- 06/30/2021, Total : \$450,000

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

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

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

## PREVIOUS FUNDING

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)

Dr. Pascal Krause (2009-2012)

Dr. Kurt A. Kistler (2010-2011)

Dr. Mariana Assmann (2013-2015)

Dr. Wook Lee (2014 -2016)

Dr. Tolga Karsili (2016 -2018)

Dr. James Brown (2016 - 2017)

Dr. Patricia Vindel Zandbergen (2018 - 2019)

Dr. Cate Anstöter (2020-present)

### **Graduate Students:**

Dr. Kurt A. Kistler (2004-2010)

10 papers + 1 review chapter published

Awarded: CST outstanding research award, the Daniel Swern Fellowship, the Case Fellowship, CST graduate student travel award, prize for poster at the Philadelphia ACS meeting, currently faculty at Penn State, Brandywine

Dr. Zhen Lu (2009-2015) (5 papers published, currently faculty at the University of Pittsburgh at Johnstown )  
Ranjeetha Suryavanshi (2008-2009)  
Dr. Vincent Spata (2011 - 2016) (5 papers published, currently a postdoc at Princeton University)  
Congyi Zhou (2009-2012) (6 papers published)  
Mark Fennimore (2014-2018)  
Pratip Chakraborty (2015-present)  
Salsabil Abou-Hatab (2017-present)  
Mushir Thodika (2017-present)  
Mohammed Sorour (2018 - present)  
Vaibhav Singh (2019-present)

### **Undergraduate Students:**

Ruth Elliott (2004-2005) (1 paper published, first author)(Diamond Scholar)  
Kandis Gilliard (2005-2006) (1 paper published) (AMP summer research scholarship, currently a graduate student at UIUC)  
Madihya Muhammad (Summer 2007)  
Benjamin Mejia (Summer 2007)  
Elizabeth Mburu (2007-2008) (1 paper published, first author) (recipient of the Clearfield and Fineman CST awards)  
Nickolas Crawford (Summer 2009)  
Christopher Kozak (2008-2010) (1 paper published, first author) (recipient of the local ACS award, currently at Dow Chemical)  
Parth Patel (Spring 2010)  
JingXin Liang (2009-2012) (2 papers published, first author) (Diamond Peer Teacher, Diamond Research scholar, received the Tomlison award, the Conwell Undergraduate Research Award, the Henry A. Slovirer Student Research Award in Chemistry, and a University Scholarship, currently a graduate student at Caltech)  
Quynh Nguyen (2012-2014) (2 papers published, NSF GRFP fellowship, currently a graduate student at Colorado Boulder)  
Catherine Triandafillou (2011-2013) (1 paper published, first author)(American Institute of Chemists (AIC) Award, NSF GRFP fellowship) (currently a graduate student at the University of Chicago)  
Stephen Meloni (Summer 2012-Spring 2014) (1 paper published, currently a graduate student at UPenn)  
Thuylinh Cao (Fall 2013 - Spring 2014)  
Dillion Fox (Spring 2014) (currently a graduate student at UPenn)  
Yang Zeng (Spring 2015)  
Aya Matsumura (Spring 2015 -Summer 2015)  
Salsabil Abou-Hatab (Spring 2015-Spring 2016)(1 paper published, currently a graduate student at Temple)  
Margaret Anne King (Summer 2016)  
Chey Jones (Fall 2014 - Spring 2017, Philadelphia Section ACS award, NSF GRFP fellowship, currently a graduate student at Stanford University)  
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) Camilo Zuluaga (Summer 2019-present)  
Drew Behrendt (Summer 2019-present)

**High School Students:**

Carina Tse (2015-2017)

Palak Shah (2017 - 2018)

Mazin Ahmed (2018)