

## PUBLICATIONS IN PEER-REVIEWED JOURNALS

(undergraduate students are underlined)

### Since joining UL Lafayette:

1. X. Lei, Q. Lian, X. Zhang, **T. N. V. Karsili**, W. Holmes, Y. Chen, M. E. Zappi, D. D. Gang, A review of PFAS adsorption from aqueous solutions: Current approaches, engineering, applications, challenges, and opportunities, *Environmental Pollution*, 2023, **321**, 121138.
2. G. Wang, T. Liu, M. Zou, C. A. Soj dak, M. C. Kozlowski, **T. N. V. Karsili**, and M. I. Lester, Electronic Spectroscopy and Dissociation Dynamics of Vinyl-Substituted Criegee Intermediates: 2-Butenal Oxide and Comparison with Methyl Vinyl Ketone Oxide and Methacrolein Oxide Isomers, *Journal of Physical Chemistry A*, 2023, **127**, 203–215.
3. E. Antwi, N. A. Packer, J. M. Ratliff, B. Marchetti, **T. N. V. Karsili**, Insights into the Ultrafast Photodissociation Dynamics of Isoprene Derived Criegee Intermediates, *Photochemistry and Photobiology*, 2022, DOI: 10.1111/php.13736.
4. E. J. Stelz-Sullivan, J. M. Racca, J. C. McCoy, D. L. Charif, L. Islam, X-D Zhou, B. Marchetti, **T. N. V. Karsili**, Enhancing STEM Education by Integrating Research and Teaching in Photochemistry: An Undergraduate Chemistry Laboratory in Spectroscopy and Photochemistry, *Education Sciences*, 2022, **12**, 729.
5. E. Antwi, J. M. Ratliff, M. N. R. Ashfold, **T. N. V. Karsili**, Comparing the Excited State Dynamics of CH<sub>2</sub>OO, the Simplest Criegee Intermediate, Following Vertical versus Adiabatic Excitation, *Journal of Physical Chemistry A*, 2022, **126**, 6236 - 6243.
6. E. Antwi, R. E. Bush, B. Marchetti, **T. N. V. Karsili**, A direct dynamics study of the exotic photochemistry of the simplest Criegee intermediate, CH<sub>2</sub>OO, *Physical Chemistry Chemical Physics*, 2022, **24**, 16724 - 16731.
7. **T. N. V. Karsili**, B. Marchetti, M. I. Lester, M. N. R. Ashfold, Electronic Absorption Spectroscopy and Photochemistry of Criegee Intermediates, *Photochemistry and Photobiology*, 2022, DOI: 10.1111/php.13665.
8. E. J. Stelz-Sullivan, B. Marchetti, **T. N. V. Karsili**, Simulating Electronic Absorption Spectra of Atmospherically Relevant Molecules: A Systematic Assignment for Enhancing Undergraduate STEM Education, *Education Sciences*, 2022, **12**, 252.
9. J. McCoy, C. F. Frey III, S. J. Leger, M. F. Vansco, B. Marchetti, **T. N. V. Karsili**, Modeling the electronic absorption spectra and photolysis rates of methyl vinyl ketone oxide and methacrolein oxide, *Journal of Physical Chemistry A*, 2022, **126**, 485-496.
10. B. Marchetti, V. J. Esposito, R. E. Bush, **T. N. V. Karsili**, The States That Hide in the Shadows: The Potential Role of Conical Intersections in the Ground State Unimolecular Decay of Criegee Intermediates, *Physical Chemistry Chemical Physics*, 2022, **24**, 532-540.

11. Y. Guan, X. Zhang, Y. Zhang, **T. N. V. Karsili**, M. Fan, Y. Liu, B. Marchetti, X-D. Zhou, Achieving high selectivity towards electro-conversion of CO<sub>2</sub> using In-doped Bi derived from metal-organic frameworks, *Journal of Colloid and Interface Science*, 2022, **612**, 235-245.
12. Y. Zhang, W. Wang, Y. Wang, N. Xu, G. Tian, **T. N. V. Karsili**, J. Yang, X-D. Zhou, Role of Pr-Vacancies and O-Interstitials on the Activity and Stability of (Pr<sub>1-x</sub>Ln<sub>x</sub>)<sub>2</sub>NiO<sub>4</sub> (Ln = La, Nd, Pm, Sm, Gd, Tb, Dy, and Ho) towards Oxygen Reduction Reactions: A DFT Study, *Journal of The Electrochemical Society*, 2021, **168**, 124508.
13. V. J. Esposito, O. Werba, S. A. Bush, B. Marchetti, **T. N. V. Karsili**, Insights into the Ultrafast Dynamics of CH<sub>2</sub>OO and CH<sub>3</sub>CHOO Following Excitation to the Bright  $1\pi\pi^*$  State: The Role of Singlet and Triplet States, *Photochemistry and Photobiology*, 2021, Accepted, DOI: 10.1111/php.13560.
14. X. Wang, M. Fan, Y. Guan, Y. Liu, M. Liu, **T. N. V. Karsili**, J. Yi, X-D Zhou, J. Zhang, MOF-based electrocatalysts for high-efficiency CO<sub>2</sub> conversion: structure, performance, and perspectives, *Journal of Materials Chemistry A*, 2021, **9**, 22710-22728.
15. G. Wang, T. Liu, A. Caracciolo, M. F. Vansco, N. Trongsirawat, P. Walsh, B. Marchetti, **T. N. V. Karsili**, and M. I. Lester, Photodissociation Dynamics of Methyl Vinyl Ketone Oxide: A four-carbon unsaturated Criegee intermediate from isoprene ozonolysis, *Journal of Chemical Physics*, 2021, **155**, 174305.
16. V. J. Esposito, T. Liu, G. Wang, A. Caracciolo, M. F. Vansco, B. Marchetti; **T. N. V. Karsili**, M. I. Lester, Photodissociation Dynamics of CH<sub>2</sub>OO on Multiple Potential Energy Surfaces: Experiment and Theory, *Journal of Physical Chemistry A*, 2021, **125**, 30, 6571–6579.
17. J. C. McCoy, B. Marchetti and **T. N. V. Karsili**, A Simple and Efficient Method for Simulating the Electronic Absorption Spectra of Criegee Intermediates: Benchmarking on CH<sub>2</sub>OO and CH<sub>3</sub>CHOO, *Journal of Physical Chemistry A*, 2021, **125**, 19, 4089–4097.
18. V. C. Frederick, T. A. Ashy, B. Marchetti, M. N. R. Ashfold and **T. N. V. Karsili**, Photoprotective Properties of Eumelanin: Computational Insights into the Photophysics of a Catechol:Quinone Heterodimer Model System, *Photochemistry*, 2021, **1**, 26–37.
19. S. J. Leger, B. Marchetti, M. N. R. Ashfold and **T. N. V. Karsili**, The Role of Norrish Type-I Chemistry in Photoactive Drugs: An ab initio Study of a Cyclopropenone-Enediyne Drug Precursor, *Frontiers in Chemistry*, 2020, accepted, DOI: 10.3389/fchem.2020.596590.
20. C. Hansen, B. Marchetti, **T. N. V. Karsili** and M. N. R. Ashfold, Ultraviolet Photodissociation of Gas-Phase Transition Metal Complexes: Dicarboxylcyclopentadienyliodoiron(II), *Molecular Physics*, 2020, accepted, DOI: 10.1080/00268976.2020.1813343.

21. J. B. Tran, J. C. McCoy, Lori M. Bailey, B. P. McDaniel, R. L. Simon, B. Marchetti and **T. N. V. Karsili**, An Affordable Set-Up for Studying Photochemistry in Action in Undergraduate Teaching Laboratories, *Journal of Chemical Education*, 2020, DOI: 10.1021/acs.jchemed.0c00354.
22. R. K. R. Singh, **T. N. V. Karsili** and R. S. Srivastava, Cooper-Catalyzed Enantioselective direct  $\alpha$ -C-H Amination of  $\beta$ -Dicarbonyl derivatives with Aryl hydroxylamines and Mechanistic Insights, *Molecular Catalysis*, 2020, DOI: 10.1016/j.mcat.2020.111067.
23. P. R. Albuquerque, R. Ramachandran, T. Junk and **T. N. V. Karsili**, Hydrogen-Deuterium Exchange in Basic Near-Critical and Supercritical Media: An Experimental and Theoretical study, *Journal of Physical Chemistry A*, 2020, **124**, 2530-2536.
24. **T. N. V. Karsili** and B. Marchetti, Oxidative Addition of singlet oxygen to model building-blocks of the Aerucyclamide A Peptide: A first principles approach, *Journal of Physical Chemistry A*, 2020, **124**, 498-504.
25. M. Thodika, M. A. Fennimore, **T. N. V. Karsili**, S. Matsika, Comparative study of methodologies for calculating metastable states of small to medium-sized molecules, *Journal of Chemical Physics*, 2019, **151**, 244104.
26. F. A. Mautner, P. Jantscher, R. Fischer, A. Torvisco, R. Vicente, **T. N. V. Karsili**, S. S. Massoud, Structure, DFT Calculations and Magnetic Characterization of Coordination Polymers of Bridged Dicyanamido-metal(II) Complexes, *Magnetochemistry*, 2019, **5**, 41.
27. P. Jantscher, R. C Fischer, A. Torvisco, R. Vicente, **T. N. V. Karsili**, S. S. Massoud, F. A. Mautner, Synthesis and characterization of 1D coordination polymers of metal(II)-dicyanamido complexes, *Polyhedron*, 2019, **167**, 39-43.
28. M. Bain, C. S. Hansen, **T. N. V. Karsili** and M. N. R. Ashfold, Quantifying rival bond fission probabilities following photoexcitation: C-S bond fission in t-butylmethylsulfide. *Chemical Science*, 2019, **10**, 5290 - 5298.
29. F. A. Mautner, R. C. Fischer, A. Torvisco, M. M. Henary, A. Milner, H. DeVillier, **T. N. V. Karsili**, F. R. Louka and S. S. Massoud, Steric Effects of Alkyl Substituents at N-Donor Bidentate Amines Directs the Nuclearity, Bonding and Bridging Modes in Thiocyanato-Copper(II) Complexes, *Crystals*, 2019, **9**, 38.
30. M. N. R. Ashfold, R. A. Ingle, **T. N. V. Karsili** and J. Zhang, Photoinduced C-H bond fission in prototypical organic molecules and radicals, *Physical Chemistry Chemical Physics*, 2019, **21**, 13880 - 13901.
31. B. Marchetti, **T. N. V. Karsili** and M. N. R. Ashfold, Photofragment Translational Exploring Norrish Type I and Type II Reactions: An ab initio Mechanistic Study Highlighting Singlet-State Mediated Chemistry, *Physical Chemistry Chemical Physics*, 2019, **21**, 14418 - 14428.

32. X. Wu, J. Ehrmaier, A. L. Sobolewski, **T. N. V. Karsili** and W. Domcke, Mechanisms of the photoreactivity of adenine in water, *Physical Chemistry Chemical Physics*, 2019, **21**, 14238-14249.
33. G. Cooper, C. Hansen, **T. N. V. Karsili** and M. N. R. Ashfold, Photofragment Translational Spectroscopy Studies of H Atom Loss Following Ultraviolet Photoexcitation of Methimazole in the Gas Phase, *Journal of Physical Chemistry A*, 2018, **122**, 9869-9878.
34. **T. N. V. Karsili**, B. Marchetti and M. N. R. Ashfold, The Role of pi-sigma\* States in the Formation of Adenine Radical-Cations in DNA Duplexes, *Chemical Physics*, 2018, **515**, 464-471.

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35. **T. N. V. Karsili**, M. Ul Hasan K T, L. Nguyen and S. Matsika, The Origin of Fluorescence in DNA Thio-Analogues, *Chemical Physics*, 2018, **515**, 434-440.
36. **T. N. V. Karsili**, M. A. Fennimore and S. Matsika, Electron-Induced Origins of Prebiotic Sugars: Self-Reactions of Methanol Anion Clusters, *Physical Chemistry Chemical Physics*, 2018, **20**, 12599-12607.
37. **T. N. V. Karsili**, B. Marchetti and S. Matsika, Origins of Photodamage in Pheomelanin Constituents: Photochemistry of 4-Hydroxybenzothiazole, *Journal of Physical Chemistry A*, 2018, **122**, 1986-1993.
38. N. D. N. Rodrigues, N. Cole-Filipiak, M. D. Horbury, M. Staniforth, **T. N. V. Karsili**, Y. Peperstraete and V. G. Stavros, Photophysics of the sunscreen ingredient menthyl anthranilate and its precursor methyl anthranilate: a bottom-up approach to photoprotection, *Journal of Photochemistry and Photobiology A*, 2018, **353**, 376-384.
39. P. Chakraborty, **T. N. V. Karsili**, B. Marchetti and S. Matsika, Mechanistic insights into photoinduced damage of DNA and RNA nucleobases in the gas phase and in bulk solution, *Faraday Discussions*, 2018, **207**, 329-350.
40. Light induced charge and energy transport in nucleic acids and proteins: general discussion, *Faraday Discussions*, 2018, **207**, 153-180
41. Photocrosslinking between nucleic acids and proteins: general discussion, *Faraday Discussions*, 2018, **207**, 283-306.
42. Light induced damage and repair in nucleic acids and proteins: general discussion, *Faraday Discussions*, 2018, **207**, 389-408.
43. Bionanophotonics: general discussion, *Faraday Discussions*, 2018, **207**, 491-512.
44. F. Adams, M. R. Machat, P. T. Altenbuchner, J. Ehrmaier, A. Pöthig, **T. N. V. Karsili** and B. Rieger, Toolbox of Nonmetallocene Lanthanides: Multifunctional Catalysts in Group-Transfer Polymerization, *Inorganic Chemistry*, 2017, **56**, 9754-9764.

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49. J. Ehrmaier, **T. N. V. Karsili**, A. L. Sobolewski and W. Domcke, On the Mechanism of Photocatalytic Water Splitting with Graphitic Carbon Nitride: Photochemistry of the Heptazine-Water Complex, *Journal of Physical Chemistry A*, 2017, **121**, 4754-4764.
50. L. A. Baker, B. Marchetti, **T. N. V. Karsili**, V. G. Stavros and M. N. R. Ashfold, Photoprotection: Extending lessons learned from studying natural sunscreens to the design of artificial sunscreen constituents, *Chemical Society Reviews*, 2017, **46**, 3770-3791.
51. B. Marchetti, **T. N. V. Karsili**, M. Cipriani, C. S. Hansen and M. N. R. Ashfold, The near ultraviolet photodissociation dynamics of 2- and 3-substituted thiophenols: Geometric vs. electronic structure effects, *The Journal of Chemical Physics*, 2017 **147**, 013923.
52. J. Ehrmaier, D. Picconi, **T. N. V. Karsili** and W. Domcke, Photodissociation dynamics of the pyridinyl radical: Time-dependent quantum wave-packet calculations, *The Journal of Chemical Physics*, 2017, **146**, 124304.
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