

PUBLICATIONS IN PEER-REVIEWED JOURNALS

(undergraduate students are underlined)

Since joining UL Lafayette:

1. Eleanor 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.
2. 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.
3. 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.
4. 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 CO₂ using In-doped Bi derived from metal-organic frameworks, *Journal of Colloid and Interface Science*, 2022, **612**, 235-245.
5. 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_{1-x}Ln_x)₂NiO₄ (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.
6. V. J. Esposito, O. Werba, S. A. Bush, B. Marchetti, **T. N. V. Karsili**, Insights into the Ultrafast Dynamics of CH₂OO and CH₃CHOO 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.
7. 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 CO₂ conversion: structure, performance, and perspectives, *Journal of Materials Chemistry A*, 2021, **9**, 22710-22728.
8. G. Wang, T. Liu, A. Caracciolo, M. F. Vansco, N. Trongsiwat, 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.
9. V. J. Esposito, T. Liu, G. Wang, A. Caracciolo, M. F. Vansco, B. Marchetti; **T. N. V. Karsili**, M. I. Lester, Photodissociation Dynamics of CH₂OO on Multiple Potential Energy Surfaces: Experiment and Theory, *Journal of Physical Chemistry A*, 2021, **125**, 30, 6571-6579.

10. 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 CH₂OO and CH₃CHOO, *Journal of Physical Chemistry A*, 2021, **125**, 19, 4089–4097.
11. 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.
12. 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.
13. C. Hansen, B. Marchetti, **T. N. V. Karsili** and M. N. R. Ashfold, Ultraviolet Photodissociation of Gas-Phase Transition Metal Complexes: Dicarboxylcyclopentadienylidodiron(II), *Molecular Physics*, 2020, accepted, DOI: 10.1080/00268976.2020.1813343.
14. 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.
15. R. K. R. Singh, **T. N. V. Karsili** and R. S. Srivastava, Cooper-Catalyzed Enantioselective direct α -C-H Amination of β -Dicarbonyl derivatives with Aryl hydroxylamines and Mechanistic Insights, *Molecular Catalysis*, 2020, DOI: 10.1016/j.mcat.2020.111067.
16. P. R. Alburquerque, 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.
17. **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.
18. 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.
19. 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.
20. 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.

21. 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.
22. 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.
23. 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.
24. 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.
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26. 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.
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29. **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.
30. **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.
31. 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.

32. 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.
33. Light induced charge and energy transport in nucleic acids and proteins: general discussion, *Faraday Discussions*, 2018, **207**, 153-180
34. Photocrosslinking between nucleic acids and proteins: general discussion, *Faraday Discussions*, 2018, **207**, 283-306.
35. Light induced damage and repair in nucleic acids and proteins: general discussion, *Faraday Discussions*, 2018, **207**, 389-408.
36. Bionanophotonics: general discussion, *Faraday Discussions*, 2018, **207**, 491-512.
37. 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.
38. M. Staniforth, W-D. Quan, **T. N. V. Karsili**, L. A. Baker, R. K O'Reilly and V. G. Stavros, A First Step Towards a Universal Fluorescent Probe: Unravelling the Photodynamics of an Amino-Maleimide Fluorophore, *Journal of Physical Chemistry A*, 2017, **121**, 6357-6365.
39. L. Lipciuc, S. H. Gardiner, **T. N. V. Karsili**, J. W. L. Lee, D. Heathcote, M. N. R. Ashfold, C. Vallance, Photofragmentation dynamics of N , N -dimethylformamide following excitation at 193 nm, *The Journal of Chemical Physics*, 2017, **147**, 013941.
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45. 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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52. B. Marchetti and T. N. V. Karsili, Theoretical insights into the photo-protective mechanisms of natural biological sunscreens: building blocks of eumelanin and pheomelanin, *Physical Chemistry Chemical Physics*, 2016, **18**, 3844-3658.
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56. B. Marchetti, **T. N. V. Karsili**, O. Kelly, P. Kapetanopoulos and M. N. R. Ashfold, *The Journal of Chemical Physics*, 2015, **14**, 224303.

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