

PUBLICATIONS IN PEER-REVIEWED JOURNALS

(undergraduate students are underlined>

Since joining UL Lafayette:

1. L. M. Guidry, S. E. Guidry, T. Barua, B. Marchetti, M. F. Vansco, and **T. N. V. Karsili**, Characterizing the Excited States and Electronic Absorption Spectra of Small Alkylperoxy ($\text{RO}_2\bullet$) and Hydroperoxy ($\bullet\text{QOOH}$) Radicals, *Photochem*, 2025, 5, 26.
2. E. Karlsson, R. Rabayah, **T. N. V. Karsili**, M. I. Lester, Electronic Spectroscopy and Characterization of the Singly Fluorinated Criegee Intermediate FCHOO, *The Journal of Physical Chemistry A*, 2025, 129, 36, 8387–8394.
3. L. M. Guidry, K. A. Zeringue, T. Barua, M. F. Vansco, B. Marchetti, and T. N. V. Karsili, Thermal and Photoinduced Chemistry of the Aromatic Criegee Intermediate, Benzaldehyde Oxide: Implications for Indoor Air Quality, *Photochemistry and Photobiology*, 2025, DOI: 10.1111/php.70029.
4. L. M. Guidry, C. A. Poirier, A. Yigiter, T. P. Legg, B. Marchetti, M. N. R. Ashfold, M. F. Vansco, and **T. N. V. Karsili**, Unraveling Electronic Effects that Influence the Bimolecular Chemistry of Fluorinated Criegee Intermediates, *ChemPhysChem*, 2025, 26, e202401023.
5. D. Timsina, D. Duong, J. M. Miller, V. Bell, **T. N. V. Karsili**, W. A. Hollerman, S. W. Allison, J. Collins, F. Sabri, Spectral analysis and characterization of several polymer encapsulated phosphor materials for sensing applications, *Optical Materials*, 2025, 166, 117116.
6. M. Zou, E. Moya Cruz, C. A. Soj dak, M. C. Kozlowski, **T. N. V. Karsili**, and M. I. Lester, UV Photodissociation Dynamics of Organic Hydroperoxides: Experiment and Theory, *The Journal of Physical Chemistry A*, 2025, 129, 13, 3052–3062.
7. E. Karlsson, R. Rabayah, T. Liu, C. A. Soj dak, M. C. Kozlowki, **T. N. V. Karsili**, and M. I. Lester, Electronic Spectroscopy of the Halogenated Criegee Intermediate, ClCHOO: Experiment and Theory, *The Journal of Physical Chemistry A*, 2024, 128, 51, 10949–10956.
8. L. M. Guidry, L. A. Bardash, A. Yigiter, S. Ravi, B. Marchetti, and **T. N. V. Karsili**, The Role of Solar Photolysis in the Atmospheric Removal of Methacrolein Oxide and the Methacrolein Oxide–Water van-der Waals Complex in Pristine Environments, *Photochemistry and Photobiology*, 2024, accepted, DOI: 10.1111/php.14007.
9. T. K. Roy, Y. Qian, E. Karlsson, R. Rabayah, C. A. Soj dak, M. C. Kozlowki, **T. N. V. Karsili**, and M. I. Lester, Vibrational spectroscopy and dissociation dynamics of cyclohexyl hydroperoxide, *Chemical Science*, 2024, 15, 6160–6167, DOI: 110.1039/D4SC00151F.

10. C. A. Poirier, L. M. Guidry, J. M. Ratliff, V. J. Esposito, B. Marchetti, and **T. N. V. Karsili**,* Modeling the Ground and Excited State Unimolecular Decay of the Simplest Fluorinated Criegee Intermediate, HFCOO, formed from the Ozonolysis of Hydrofluoroolefin Refrigerants, *Journal of Physical Chemistry A*, 2023, DOI: 10.1021/acs.jpca.3c01530.
11. L. M. Guidry, C. A. Poirier, J. M. Ratliff, E. Antwi, B. Marchetti*, **T. N. V. Karsili**,* Modeling the Unimolecular Decay Dynamics of the Fluorinated Criegee Intermediate, CF₃CHOO, *Photochem*, 2023, 3(3), 327-335.
12. G. Wang, T. Liu, M. Zou, **T. N. V. Karsili**,* and M. I. Lester*, UV photodissociation dynamics of the acetone oxide Criegee intermediate: experiment and theory, *Physical Chemistry Chemical Physics*, 2023, 25, 7453-7465.
13. 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.
14. 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.
15. 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*, 2023, **99**, 1072-1079.
16. **T. N. V. Karsili**,* B. Marchetti, M. I. Lester, M. N. R. Ashfold, Electronic Absorption Spectroscopy and Photochemistry of Criegee Intermediates, *Photochemistry and Photobiology*, 2023, **99**, 4-18.
17. 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.
18. E. Antwi, J. M. Ratliff, M. N. R. Ashfold, **T. N. V. Karsili**,* Comparing the Excited State Dynamics of CH₂OO, the Simplest Criegee Intermediate, Following Vertical versus Adiabatic Excitation, *Journal of Physical Chemistry A*, 2022, 126, **36**, 6236 - 6243.
19. E. Antwi, R. E. Bush, B. Marchetti, **T. N. V. Karsili**,* A direct dynamics study of the exotic photochemistry of the simplest Criegee intermediate, CH₂OO, *Physical Chemistry Chemical Physics*, 2022, **24**, 16724 - 16731.
20. 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.

21. 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.
22. 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.
23. 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.
24. 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.
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26. 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.
27. 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.
28. 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.
29. J. C. McCoy, B. Marchetti, M. U. Thodika, 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.
30. 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.

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32. C. Hansen, B. Marchetti, **T. N. V. Karsili** and M. N. R. Ashfold,* Ultraviolet Photodissociation of Gas-Phase Transition Metal Complexes: Dicarboxylcyclopentadienyliron(II), *Molecular Physics*, 2020, accepted, DOI: 10.1080/00268976.2020.1813343.
33. 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.
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35. 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.
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46. **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.

Prior to joining UL Lafayette:

47. **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.
48. **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.
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