

Full List of Publications

1. 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, *J. Phys. Chem. A*, 2020, accepted.
2. 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, *J. Phys. Chem. A.*, 2020, 124, 498-504.
3. 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, *J. Chem. Phys.*, 2019, 151, 244104.
4. 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.
5. 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 *tert*-butylmethylsulfide, *Chem. Sci.*, 2019, 10, 5290-5298.
6. F. A. Mautner, P. Jantscher, R. C. Fischer, A. Torvisco, R. Vincente, T. N. V. Karsili, S. S. Massoud, Synthesis and characterization of 1D coordination polymers of metal(II)-dicyanamido complexes, *Polyhedron*, 2019, 167, 39-43.
7. Marchetti, T. N. V. Karsili and M. N. R. Ashfold, Exploring Norrish Type I and Type II Reactions: An *ab initio* Mechanistic Study Highlighting Singlet-State Mediated Chemistry, *Phys. Chem. Chem. Phys.*, 2019, 21, 14418-14428. (invited special issue on photodissociation and reaction dynamics).
8. 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.
9. 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, *Phys. Chem. Chem. Phys.*, 2019, 21, 13880-13901 (invited special issue on photodissociation and reaction dynamics).
10. 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, *J. Phys. Chem. A.*, 2019, 122, 9869-9878.

11. X. Wu, J. Ehrmaier, A. L. Sobolewski, T. N. V. Karsili and W. Domcke, Mechanisms of the photoreactivity of adenine in water, *Phys. Chem. Chem. Phys.*, 2019, 21, 14238-14249. (invited special issue on photodissociation and reaction dynamics).
12. T. N. V. Karsili, B. Marchetti and M. N. R. Ashfold, The Role of $^1\pi\sigma^*$ States in the Formation of Adenine Radical-Cations in DNA Duplexes, *Chem. Phys.* 2018, 515,464-471.
13. T. N. V. Karsili, M. Thodika, L. Nguyen and S. Matsika, The Origin of Fluorescence in DNA Thio-Analogues. *Chem. Phys.*, 2018, 515, 434-440.
14. T. N. V. Karsili, M. A. Fennimore and S. Matsika, Electron-Induced Origins of Prebiotic Sugars: Self-Reactions of Methanol Anion Clusters, *Phys. Chem. Chem. Phys.*, 2018, 20, 12599-12607
15. T. N. V. Karsili, B. Marchetti and S. Matsika, Origins of Photodamage in Pheomelanin Constituents: Photochemistry of 4-Hydroxybenzothiazole, *J. Phys. Chem. A*, 2018, 122, 8, 1986-1993
16. 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 Discuss.*, 2018, 207, 329-350.
17. 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, *J. Photochem Photobiol A*, 2018, 353, 376-384.
18. F. Adams, M. R. Machat, P. T. Altenbuchner, J. Ehrmaier, A. Pothig, T. N. V. Karsili and B. Rieger, Toolbox of Nonmetallocene Lanthanides: Multifunctional Catalysts in Group-Transfer Polymerization, *Inorg. Chem.*, 2017, 56, 9754-9764
19. 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, *J. Phys. Chem. A*, 2017, 121, 6357-6365.
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22. M. A. Fennimore, T. N. V. Karsili and S. Matsika, Mechanisms of H and CO Loss from the Uracil Nucleobase Following Low Energy Electron Irradiation, *Phys. Chem. Chem. Phys.*, 2017, 19, 17233-17241.
23. 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, *J. Phys. Chem. A*, 2017, 121, 4754-4764.
24. 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, *Chem. Soc. Rev.*, 2017, 46, 3770-3791.
25. 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, *J. Chem. Phys.*, 2017 147, 013923.
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27. X. Wu, T. N. V. Karsili and W. Domcke, Role of Electron-Driven Proton-Transfer Processes in the Ultrafast Deactivation of Photoexcited Anionic 8-oxoGuanine-Adenine and 8-oxoGuanine-Cytosine Base Pairs, *Molecules*, 2017, 22, 135.
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32. X. Wu, T. N. V. Karsili and W. Domcke, Excited-State Deactivation of Adenine by Electron-Driven Proton-Transfer Reactions in Adenine-Water Clusters: A Computational Study, *ChemPhysChem*, 2016, 17, 1298-1304.

33. B. Marchetti and T. N. V. Karsili, Theoretical insights into the photo-protective mechanisms of natural biological sunscreens: building blocks of eumelanin and pheomelanin, *Phys. Chem. Chem. Phys.*, 2016, 18, 3844-3658.
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39. L. A. Baker, M. D. Horbury, S. E. Greenough, P. M. Coulter, T. N. V. Karsili, G. M. Roberts, A. J. Orr-Ewing, M. N. R. Ashfold and V. G. Stavros, Probing the Ultrafast Energy Dissipation Mechanism of the Sunscreen Oxybenzone after UVA Irradiation, *J. Phys. Chem. Lett.*, 2015, 6, 1363-1368.
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41. S. H. Gardiner, M. L. Lipciuc, T. N. V. Karsili, M. N. R. Ashfold and C. Vallance, Dynamics of the A-band ultraviolet photodissociation of methyl iodide and ethyl iodide via velocity-map imaging with 'universal' detection, *Phys. Chem. Chem. Phys.*, 2015, 17, 4096-4106.
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51. D. Murdock, S. J. Harris, T. N. V. Karsili and I. P. Clark, M. Towrie, A. J. Orr-Ewing and M. N. R. Ashfold, Photofragmentation Dynamics in Solution Probed by Transient IR Absorption Spectroscopy: $\pi\sigma^*$ -Mediated Bond Cleavage in p -Methylthiophenol and p -Methylthioanisole, *J. Phys. Chem. Lett.*, 2012, 3, 3715-3720.
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