

Education

Ph.D. Physics, University of Paris Est, France & University of Tunis El-Manar, Tunisia, 2016

M.Sc., Condensed Matter Physics, University of Tunis El-Manar, Tunisia, 2012

Bachelor, Sc., University of Tunis El-Manar, Tunisia, 2010

Professional Experience

Research Associate

University of Pennsylvania, July-2023-Present

- Investigating the water and sulfur dioxide depletion in Venus' Atmosphere using computational tools.

Postdoctoral Research Associate

University of Pennsylvania, 2018-2023

- Conducted a comprehensive analysis of the pivotal role of photochemistry in the proposed solar geoengineering strategy, focused on mitigating Earth's temperature. Successfully introduced an alternative photochemical pathway to clarify the processes involving molecule destruction and the generation of new molecules.
- Successfully investigated the thermodynamics and spectroscopic properties of 11 novel aluminum compounds that were previously inaccessible to experimental studies. My groundbreaking research led to the experimental observation of two of these compounds, validating the accuracy of the predicted data.
- Accomplished comprehensive exploration of the electronic structure and thermodynamics within a diverse set of 32 molecules encompassing both organic and inorganic compounds of small and medium size. These molecules are of paramount significance to biological, atmospheric and astrophysical contexts.
- Published research findings in scientific journals and presented at national and international conferences.
- Mentored and trained graduate and undergraduate students, providing guidance in computational techniques.

Postdoctoral Fellow

University of Nebraska Lincoln, 2016-2018

- Explored the photochemistry and excited states of molecules with astronomical and astrophysical significance.
- Collaborated closely with experimental team to confirm the detection of novel gas-phase species.

Mentor & Tutor

Astronomical Society of Tunisia, 2014-present

- Provided guidance to schoolteachers and animators on effectively communicating intricate astronomical phenomena and events to the broader public. My focus was on helping them develop the skills and techniques necessary to present complex scientific concepts in a clear manner, allowing young audiences to grasp and appreciate the wonders of the cosmos more easily.

Graduate Research Assistant

University of Paris Est Marne La-Vallee, 2013-2016

- Pioneered a groundbreaking photochemical mechanism aimed at explaining the photoproduction of nitric oxide from thionitrites, which act as crucial vasodilation reservoirs in biological environments. This achievement involved a comprehensive investigation of the structural and spectroscopic properties of diverse intermediate species, including both neutral and negatively charged entities.
- Developed an innovative computational strategy that combines mono and multireference approaches, enabling a thorough exploration of the photochemical pathways of small negative anions. This breakthrough in computational methodology allows for a comprehensive understanding of the intricate photochemical processes governing these species.

Lecturer

University of Tunis El-Manar, 2012- 2013

- Department of Physics, University of Tunis El-Manar

Research Visits

- Mars-April 2016, Institut des Sciences moléculaire, Bordeaux, France *Host: Thierry Stoecklein*

Scientific Work

- Collaborated with experimental and theoretical groups for the research projects.
- Referee for the International conference and exhibition for science (ICES2023).
- Referee for Astrophysical Journal Supplement Series.
- Referee for the Journal Frontiers in Chemistry.
- Referee for the Journal of Physical Chemistry A.
- Referee for the Journal of the American Chemical Society.
- Referee for the Journal Molecules.

Student Supervision

- Supervisor of undergraduate student Juliette Lipson (University of Pennsylvania, January 2023-June2023)
- Supervisor of undergraduate student Jacqueline Friskey (University of Pennsylvania June 2020-2022)
- Co-supervision of PhD thesis of Vincent. J. Esposito (University of Pennsylvania 2019-2022)
- Co-supervision of PhD thesis of Tongheng Chen (University of Pennsylvania 2019-2020)
- Supervisor of undergraduate student Natasa Rohacs (University of Pennsylvania, March to December 2019)
- Co-supervision of PhD thesis by Bilel Mehnen (University of Tunis El-Manar 2016-2018)

Courses Taught

Mathematics for Physics (Tunisia-2012-2013)

Introductory Physics (Tunisia 2012-2013)

Technical Expertise

Programming Language: Fortran, Bash, Latex, Python (Pandas, Matplotlib, NumPy, jupyter notebook).

Computational Expertise: Mono-reference and multireference quantum chemical calculations (DFT and ab initio), Photochemistry, Potential Energy Surfaces, ab-initio Non-Adiabatic Molecular Dynamic (AINAMD), Born-Oppenheimer Molecular Dynamic simulations (BOMD), High Performance Computing (HPC).

Computational Software: MOLPRO, Gaussian09/16, Quantum Espresso, VASP, Psi4, ORCA, MOLSCAT, MOLCAS, GAMESS, CP2K, SHARC, Data Visualization (Gnuplot, Iqore-Pro, Molden, Gauss View, Gabedit)

Conference, Seminars and Talks

- Climate Change Solutions and Computational Chemistry, Riyadh, Saudi Arabia, 21th January, 2024 (**Invited Speaker**)
- Density Functional Theory, Winter School, Tunis, Tunisia, 19th-21th December, 2022 (**Invited Speaker**)
- Spectroscopic characterization of the [H, P, S, O] molecular system and chemical insights into the non-detection of phosphorus and sulfur diatomic molecules PS and PH (ISMS June 2022) Illinois USA ([contributed talk](#))
- Photochemical reactivity of atmospheric sulfur compounds of interest in solar geoengineering (2nd Workshop for Young Researchers in Chemistry May 2022) Spain ([contributed talk](#))
- Deep Insight into the Photodissociation of OSSO: (APS meeting March 2021) USA ([Invited speaker](#))
- Photochemistry of HOSO and HOSO⁺: Implication for Climate Geoengineering (ACS Virtual meeting August 2020) USA ([Talk](#))
- Astrochemistry winter school 2020 Biosphere 2 Arizona USA ([Workshop](#))
- Spectroscopy of Jupiter's Atmosphere: Insights from DFT and ab-initio calculations. International Symposium on Molecular Spectroscopy June 2019 USA ([Talk](#))
- Accurate Structure and Spectroscopy of small molecular systems of astrophysical interest, ACS meeting New-Orleans March 2018 USA ([Talk](#))
- On the role of HNS and HSN as light-sensitive NO-donors for delivery in biological media. Quantum dynamics in molecular systems: theory, modelling, simulation 9th-13th November 2015 France ([Poster](#))
- Characterization and reactivity of the weakly bound complexes [H, N, S]⁻. MOLIM 1st General Meeting 27th-29th August 2015) France (**Poster**)
- Études théoriques des états excités des systèmes HNS^q/HSN^q (q=-1, 0, +1)". Ecole de corrosion: EC2EAQ Fes 17th - 19th Décembre -2014. Morocco (**Poster**)
- Séminaire sur la Dynamique Moléculaire Sousse 26th -27th October 2013 (**Talk**) **Tunisia**
- Ten years of NET 45 Faculte des Sciences de Tunis 07th -11th December 2012 **Tunisia**

Peer-Reviewed Articles (**undergraduate** & **PhD** student coauthors)

- 76 **T.Trabelsi**, J.Lipson and JS Francisco "ClSO and ClSO₂ Photochemistry: Implication for the Venusian Atmosphere" J.Chem.Phys (Submitted)
- 75 **T.Trabelsi**, JS Francisco "Exploring the photochemistry of OAlOH: Photodissociation pathways and electronic spectra" J. Chem. Phys. 160,204304 (2024)
- 74 L Wang, X Jiang, B Sun, **T.Trabelsi**, JS Francisco, X Zeng, M Zhou, "Spectroscopy and Photochemistry of [Al, N, C, O, H]: Connectivity to Aluminium-Bearing Species in the Universe" (*Just accepted*)
- 73 J Xue, X Shao, J Li, J Li, **T.Trabelsi**, J.S Francisco, X Zeng "Observation of the Water-HNSO₂ Complex" JACS,146,5455,(2024)
- 72 D.F. Yuan, Y. Liu, **T. Trabelsi**, Y.R. Zhang, J. Li, J.S. Francisco, H. Guo and L.S. Wang "Probing the dynamics and bottleneck of the key atmospheric SO₂ oxidation reaction by the hydroxyl radical" **PNAS**, 121, N6 (2024)
- 71 L. Wang, X. Jiang, **T. Trabelsi**, G. Wang, J.S. Francisco, X. Zeng and M. Zhou "Spectroscopic Study of [Mg,H,N,C,O] Species: Implications for the Astronomical Magnesium Chemistry" **J. Am. Chem. Soc** Just accepted (2024)
- 70 W. Chen, **T. Trabelsi**, X. Xu and J.S. Francisco "Spectroscopy of triatomic [Si,O,P] molecules" **Mol. Spec.** 122,e2292166, (2023)
- 69 **T. Trabelsi**, V.J. Esposito and J. S. Francisco "Spectroscopy and Photochemistry of Aluminum-Bearing Species in the Universe" **Accounts of Chemical Research** 56,3045(2023)
- 68 **T.Trabelsi** and J.S. Francisco" Spectroscopic Characterization of [H,Cl,S,O] Molecular System : Potential Candidate for Detection in Venus Atmosphere" **J. Chem. Phys.** 158,174307,2023
- 67 **T. Trabelsi**, O. Sghaier, H. Ferjani and J.S. Francisco "Excited states and photodissociation mechanism of HMgNC and HMgCN" **Astron. Astrophys.** 672, A79, (2023)
- 66 **T. Trabelsi**, **V.J. Esposito** and J.S. Francisco "Vibrational, rotational and electronic spectroscopy for possible interstellar detection of AlNH₂ and HAlNH" **The Astrophysical Journal** 949,55, (2023)
- 65 X. Li, B. Lu, J. Jiang, L. Wang, **T. Trabelsi**, J. S Francisco, W. Fang, M. Zhou, X. Zeng "Water Complex of Imidogen" **J. Am. Chem. Soc.** 145,1982 (2023)
- 64 **J.E. Lipson**, **T. Trabelsi**, J.S Francisco "Spectroscopy and photochemistry of ClSSO" **J. Chem. Phys.** 158,024302(2023)

- 63 J. M Friskey, V. J Esposito, T. Trabelsi, J. S Francisco "Spectroscopic Properties of the Astrochemical Molecules [Al,O,Si]_x (x=0,+1)" **The Astrophysical Journal** 938,156(2022)
- 62 T.Trabelsi & J.S. Francisco "Ground state spectroscopy and photochemistry of HALOH" **J.Chem.Phys.** J. Chem. Phys. 157,12 (2022)
- 61 H. V. L. Nguyen, K. J Koziol, T. Trabelsi, S. Khemissi, M. Schwell, J. S. Francisco, I. Kleiner "Discovery of a Missing Link: First Observation of the HONO-Water Complex" **J. Phys. Chem. Lett** 13,8648(2022)
- 60 X. Li, B. Lu, L. Wang, J. Hue, B. Zhu, T.Trabelsi and J.S. Francisco " Unravelling Sulfur Chemistry in Interstellar Carbon Oxide Ices" **Nature Communications** 13(1),7150 (2022)
- 59 D. Yuan, T.Trabelsi, Y.R. Zhang, J.S. Francisco and L. Wang "Probing the Electronic structure and Bond Dissociation of SO₃ and SO₃⁻ Using High Resolution Cryogenic Photoelectron Imaging" **J. Am. Chem. Soc** 144,13740 (2022)
- 58 A.F.Monerris, J.C. Garcia, T. Trabelsi, A.S. Lopez, J. Lyons, J.S. Francisco and D. R. Sanjuan "Photochemical and thermochemical pathways to S₂ and polysulfur formation in the atmosphere of Venus" **Nature Communications** 13, 1-8 (2022)
- 57 V.J Esposito, T. Trabelsi and J. S. Francisco "AlOSO: Spectroscopy and structure of a new Group of Astrochemical Molecules" **The Astrophysical Journal** 930,29 (2022)
- 56 C. A.Cuevas, R.P. Fernandez, D.E. Kinnison, Q.Li, J.F. Lamarque, T.Trabelsi, J.S. Francisco, S.Solomon and A.S.Lopez "The influence of iodine on the Antarctic stratospheric ozone hole" **PNAS** 119,7 2022
- 55 Z. Wu, X. Shao, B.Zhu, B. Lu, T.Trabelsi, J.S. Francisco and X.Zeng "Spectroscopic characterization of two peroxy radicals during the O₂-oxidation of the methylthio radical" **Communication Chemistry**, 5,1,2022.
- 54 V.J. Esposito, T. Trabelsi and J. S. Francisco "Spectroscopic Properties Relevant to Astronomical Laboratory Detection of MCH and MCH⁺ (M=Al,Mg)" **The Astrophysical Journal** 924,139 2022
- 53 V.J. Esposito, J. Friskey T. Trabelsi and J. S. Francisco "Astrochemical significance and spectroscopy of tetratomic [H,P,S,O]" **A&A** 659,A54 (2022)
- 52 J. C. García, T. Trabelsi, A. Francés-Monerris, C. A Cuevas, A. Saiz-Lopez, D. Roca-Sanjuán, J. S Francisco "Photochemistry of HOSO₂ and SO₃ and Implications for the Production of Sulfuric Acid" **J. Am. Chem. Soc.** 143,18794 (2021)
- 51 J.C. Garcia, A.F. Monerris, C.A. Cuevas, T.Trabelsi A.S. Lopez, J.S. Francisco and D. R. Sanjuan. "Photochemistry and Non-adiabatic Photodynamic of the HOSO Radical" **J. Am. Chem. Soc.** 143,10836 (2021)
- 50 V.J . Esposito, T. Trabelsi and J. S. Francisco "Photochemistry of NH₂NO₂ and Implications for Chemistry in the Atmosphere" **J. Chem. Phys.** 154, 194301(2021)
- 49 B. Lu, T.Trabelsi, V.J. Esposito, R.C. Fortenberry, J.S. Francisco and X. Zeng "Spectroscopic Characterization of HSO₂ and HOSO Intermediates Involved in SO₂ Geoengineering" **J. Phys. Chem. A** 125, 10615 (2021)
- 48 N. Lu, V. Elakkat, J.S. Thrasher, X. Wang, E. Tessema, K. ChanR.J. Wei, T. Trabelsi and J.S. Francisco, Neutron diffraction study of significant sp³ and sp² C-H bond shortening in a fluorinated pyridinium sacharinate" **J. Am. Chem. Soc.** 143, 5550-5557 (2021)
- 47 B. Zhu, Z. Wu, L. Wang, B.Lu, T. Trabelsi, J. S. Francisco and Z. Zeng "Matrix-isolated trifluoromethylthiyl radical: Sulfur atom transfer, isomerization and oxidation reactions" **Phys. Chem. Chem. Phys.** 57 12143 (2021)
- 46 V.J. Esposito, T. Trabelsi, N. Rohacs and J. S. Francisco "Spectroscopic characterization of the first and the second excited state of the HOSO radical" **J. Phys. Chem. A** 125, 6254-6262 (2021)
- 45 T. Trabelsi, J. Plane and J.S. Francisco "Astrochemical Significance of the P+ SO Reaction: Spectroscopic Characterization of SPO, PSO and SOP isomers" **The Astrophysical Journal** 909, 122, (2021)
- 44 R.C. Fortenberry, T. Trabelsi and J.S.Francisco "Theoretical Rovibrational Characterization of HALNP: Weak Bonding but Strong Intensities" **Journal of Molecular Spectroscopy** 377,111422, (2021)
- 43 M. Kumar, T. Trabelsi, J. C. Gómez Martín, A. Saiz-Lopez, J. S Francisco "HIOx-IONO₂ Dynamics at the Air-Water Interface: Revealing the Existence of a Halogen Bond at the Atmospheric Aerosol Surface" **J. Am. Chem. Soc.** 142,12467 (2020)
- 42 X. Chu, W. Qian, B. Lu, L. Wang, J. Qin, J. Li, G. Rauhut, T. Trabelsi, J. S Francisco, X. Zeng "The Triplet Hydroxyl Radical Complex of Phosphorus Monoxide" **Angew. Chem. Int. Ed** 132, (2020) 22133-22137.
- 41 V. J. Esposito, T. Trabelsi, J. S. Francisco "High-level Ab Initio Studies of the Spectroscopic Properties of Triatomic [Al, S, O]_x (x= 0, + 1) and Its Potential for Detection in Space" **The Astrophysical Journal** 903, 71, (2020)
- 40 L. Wang, Z. Wu, B. Lu, A. K Eckhardt, P. R Schreiner, T. Trabelsi, J. S Francisco, Q. Yao, C. Xie, H. Guo, X. Zeng "Spectroscopic Identification of the SSNO Isomers" **J. Chem. Phys.** 153, 94303 (2020)
- 39 T. Chen, Z. Wan, T. Trabelsi, C. Zhu, J. S Francisco "Mechanisms of Acid-Promoted N₂ and N₂O Generation from NH₂NO and NH₂NO₂" **J. Phys. Chem A**, 124, 7575 (2020)
- 38 R. C Fortenberry, T. Trabelsi, J. S Francisco "Anharmonic Frequencies and Spectroscopic Constants of OAlOH and AlOH: Strong Bonding but Unhindered Motion" **J. Phys. Chem. A** 124, 8834 (2020) **Inside Back Cover**
- 37 V. P. Barber, V. J Esposito, T. Trabelsi, A.S. Hansen, T.A. McHenry, J.S. Francisco, and M.I. Lester, "Experimental and Computational Investigation of Vinox and 1-Methylvinox Radicals from the Unimolecular Decay of Alkyl-Substituted Criegee Intermediates" **Chem. Phys. Lett.** 751, 137478 (2020)

- 36 M. Vasiliu, **T. Trabelsi**, J. S. Francisco, K. O. Christe, D. A. Dixon "Energetic Properties, Spectroscopy, and Reactivity of NF_3O^+ " **J. Phys. Chem A**, 124, 5237 (2020)
- 35 **T. Trabelsi**, **N. Rohacs** and J.S. Francisco "Photochemistry from low-lying states of HOSO^+ " **J. Chem. Phys.** 152 (13), 134302(2020)
- 34 C. Chen, B. Lu, X. Zhao, W. Qian, j. Liu, **T. Trabelsi**, J. S Francisco, J. Qin, J. Li, L. Wang, X. Zeng "Capture of the Sulfur Monoxide–Hydroxyl Radical Complex ($\cdot\text{OH} \cdots \text{OS}$)" **J. Am. Chem. Soc.** 141,8698 (2020)
- 33 **T. Trabelsi** and J.S. Francisco "Spectroscopic characterization of the first excited state and photochemistry of the HO_3 radical" **J. Chem. Phys.** ,153, 064304 (2020)
- 32 . A. Saiz-Lopez, A. Acuna, **T. Trabelsi**, J. Carmona-García, J. Davalos D. Rivero, C. Cuevas, D. Kinnison, S. Sitkiewicz, D. Roca-Sanjuán, J.S. Francisco "Gas-phase photolysis of $\text{Hg}(\text{I})$ radical species: a new atmospheric mercury reduction process." **J. Am. Chem. Soc.** 141,8698 (2019)
- 31 B.Lu, C.Song, **T. Trabelsi**, J.S. Francisco, L. Wang, and X. Zeng "Dihalogenated Methylperoxy Radicals: Spectroscopic Characterization and Photodecomposition by Release of HO^+ " **Chem. Eur. J.** 26,2817(2020)
- 30 **T. Trabelsi** and J.S. Francisco "Photochemistry of HOSO Radical in Gas Phase" **J. Chem. Phys.** 151 (11), 111103(2019)
- 29 **T. Trabelsi**, M.C. Davis, R.C. Fortenberry, J.S. Francisco." Spectroscopic Investigation of $[\text{Al,N,C,O}]$ Refractory Molecules" **J. Chem. Phys.** 151, 244303 (2019)
- 28 R. Fortenberry, **T. Trabelsi**, B. Westbrook, W. D. Rio, and J.S. Francisco. "Molecular Oxygen Generation from the Reaction of Water Cations with Oxygen Atoms" **J. Chem. Phys.** , 150, 201103 (2019)
- 27 **T. Trabelsi**, K. Mahjoubi, **B. Mehnen**, M. Hochlaf and J.S. Francisco "Spectroscopy and characterization of AlNX ($\text{X}=\text{O}$ and S): Triatomic circumstellar molecules" **J. Chem. Phys** 150,124306 (2019)
- 26 Z. Wu, C. Chen, J. Liu, Y. Lu, J. Xu, X. Liu, G. Cui, **T. Trabelsi**, J. S. Francisco, A. Mardyukov, A. K Eckhardt, P. R Schreiner, X. Zeng. "Caged Nitric Oxide-Thiyl Radical Pairs" **J. Am. Chem. Soc.** 141,3361 (2019)
- 25 **T. Trabelsi**, K. Mahjoubi, **B. Mehnen**, M. Hochlaf and J.S. Francisco "Spectroscopy and Stability of AlOP^+ : A Possible Progenitor of Interstellar Metal" **J. Phys. Chem. A** 123,463 (2018).
- 24 **T. Trabelsi** and J.S. Francisco," Is AlOH the astrochemical reservoir molecule of AlO ? Insights from excited electronic states" **The Astrophysical Journal** 863,139(2018).
- 23 W., Zhuang, C. Song, J. Liu, B. Lu, Y. Lu, **T. Trabelsi**, J. S. Francisco, and X. Zeng "Photochemistry of OPN^+ : Formation of Cyclic PON and Reversible Combination with Carbon Monoxide" **Chem. Eur. J.** 24,14627(2018)
- 22 T. Stoecklin, P. Halvick, M.d.J.Lara-Moreno, **T. Trabelsi** and M. Hochlaf "On the gas-phase formation of the HCO^- anion: Accurate quantum study of the $\text{H}^- + \text{CO}$ radiative association and HCO radiative electron attachment" **Faraday Discussion** 10.1039/C8FD00103K (2018).
- 21 **T. Trabelsi**, Y. Ajili, K. Hammami, M. Hochlaf and J.S. Francisco "The rotational excitation of $\text{SN}^+(\text{X}^1\Sigma^+)$ by collision with He at low temperature" **MNRAS** 480,4259(2018).
- 20 J. Xu, Z. Wu, H. Wan, G. Deng,¹ B. Lu, A. K. Eckhardt, P. R. Schreiner, **T. Trabelsi**, J. S. Francisco, and X. Zeng "Phenylsulfinyl Radical: Gas-phase Generation, Photoisomerization, and Oxidation" **J. Am. Chem. Soc.** 140,9972(2018).
- 19 **T. Trabelsi**, M.M. Al-Mogren, M. Hochlaf and J.S. Francisco "Mechanistic study of the photoexcitation, photoconversion and photodissociation of CS_2 " **J. Chem. Phys.** 149,64304(2018)
- 18 **T. Trabelsi**, M. Hochlaf and J.S. Francisco "Toward the detection of the triatomic negative ion SPN^- : Spectroscopy and potential energy surface. " **J. Chem. Phys** 148,164305(2018)
- 17 R. Fortenberry, **T. Trabelsi** and J.S. Francisco "Hydrogen sulfide as a scavenger of sulfur atomic cation" **J. Phys. Chem. A** 122,4983(2018)
- 16 X. Dong, G. Deng, J. Xu, B. Lu, Z. Wu, **T. Trabelsi**, J. S. Francisco, X. Zeng " Generation and Spectroscopic Identification of H_2NSO and syn- and anti- HNSOH^+ " **Angew. Chem. Int. Ed** 57 (2018) 7513-7517
- 15 **T. Trabelsi**, M.M. Al-Mogren, M. Hochlaf and J.S. Francisco "Electronic and spectroscopic characterizations of SNP isomers" **J. Chem. Phys.** 148,54305 (2018)
- 14 Z. Wu, R. Feng, J. Xu, Y. Lu, B. Lu, T. Yang , G. Frenking, **T. Trabelsi**, J.S. Francisco and X.Zeng "Photoinduced Sulfur-Nitrogen Bond Rotation and Thermal Nitrogen Inversion in Heterocumulene OSNSO^+ " **J. Am. Chem. Soc.** 140, 1231-1234 (2018).
- 13 O Denis-Alpizar, **T. Trabelsi**, M. Hochlaf, T. Stoecklin "Rotational relaxation of $\text{AlO}^+(\text{X}^1\Sigma^+)$ in collision with He " **MNRAS** 475, 783-787 (2018).
- 12 Z. Wu, J. Xu, L. Sokolenko, Y.L. Yagupolskii, R. Feng, Q. Liu, Y. Lu, L. Zhao, I. Fernandez, G. Frenking, **T. Trabelsi**, J.S. Francisco and X.Zeng "Parent Thioketene S-Oxide H_2CCSO : Gas-Phase Generation, Structure, and Bonding Analysis" **Chem. Eur. J.** 23 (2017) 16566-16573 .
- 11 Z. Wu, J. Xu, G. Deng, X. Chu, L. Sokolenko, **T. Trabelsi**, J.S. Francisco, A.K. Eckhardt, P. R. Schreiner and X. Zeng, "The Trifluoromethyl Sulfinyl and Oxathiyl Radicals" **Chem. Eur. J.** 24(7), 1505-1508 (2018).
- 10 C.T. Bop, **T. Trabelsi**, K. Hammami, M. Al-Morgen, F. Lique and M. Hochlaf "Cold collision of SH^- with He : Potential energy surface and rate coefficients" **J. Chem. Phys.** 147,124301(2017)
- 9 **T. Trabelsi**, M.Kumar and J.S. Francisco, " Substituent effects on the spectroscopic properties of Criegee intermediates" **J. Chem. Phys.** 147,164303(2017).

- 8 **T. Trabelsi**, M. Kumar and J.S. Francisco, " How Does the Central Atom Substitution Impact the Properties of Criegee Intermediate? Insights from Multi-Reference Calculations. " **J. Am. Chem. Soc.** **139**,15446(2017).
- 7 Z. Wu, J. Xu, Q. Liu, X. Dong, D. Li, N. Holtzman, G. Frenking, **T. Trabelsi**, J.S. Francisco and X. Zeng " The hypothiocyanite radical OSCN and its isomers" **Phys. Chem. Chem. Phys.** **19**,16713 (2017).
- 6 Z Wu, Q Liu, J Xu, H Sun, D Li, C Song, DM Andrada, G. Frenking, **T. Trabelsi**, J.S. Francisco and X.Zeng. "Heterocumulene Sulfinyl Radical OCNSO" **Angew. Chem. Int. Ed** **129**, 2172(2017)
- 5 Y Ajili, **T. Trabelsi**, O Denis-Alpizar, T Stoecklin, AG Császár, M Mogren Al-Mogren, JS Francisco, M Hochlaf "Vibrational memory in quantum localized states" **Phys. Rev. A** **93**,052514 (2016).
- 4 **T. Trabelsi**, S. Ben Yaghlane, N.-E. Jaidane, M. Al-Mogren, J. S. Francisco and M. Hochlaf "HNS⁺ and HSN⁺ cations: Electronic states, spin-rovibronic spectroscopy with planetary and biological implications" **J. Chem. Phys.** **145**, 084307 (2016).
- 3 **T. Trabelsi**, O. Yazidi, J. S. Francisco, R. Linguerri, and M. Hochlaf. "Electronic structure of NSO⁻ and SNO⁻ anions: Stability, electron affinity and spectroscopic properties". **J. Chem. Phys.** **143**, 164301 (2015).
- 2 **T. Trabelsi**, R. Linguerri, S. Ben Yaghlane, N.-E. Jaidane, M. Al-Mogren, J. S. Francisco and Hochlaf. "On the Role of HNS and HSN as Light-Sensitive NO-Donors for Delivery in Biological Media". **J. Chem. Phys.** **143**, 134301 (2015).
- 1 **T. Trabelsi**, Y. Ajili, S. Ben Yaghlane, N.-E. Jaidane, M. Al-Mogren, J. S. Francisco and M. Hochlaf."Characterization and reactivity of the weakly bound complexes of the [H, N, S]⁻ anionic system with astrophysical and biological implications". **J. Chem. Phys.** **143**, 034303 (2015)