

EDUCATION

Ph.D. Physics, University of Paris Est, France & University of Tunis El-Manar, Tunisia, 2012-2016
M.Sc., Condensed Matter Physics, University of Tunis El-Manar, Tunisia, 2010-2012
B.Sc., University of Tunis El-Manar, Tunisia, 2006-2010

PROFESSIONAL EXPERIENCE

Research Associate **University of Pennsylvania**, July-2023-Present

- Studying the near-UV absorber, an enigma in Venus's atmosphere.

Postdoctoral Research Associate **University of Pennsylvania**, 2018-2023

- I investigated the photochemical mechanisms of critical atmospheric and astrochemical molecules, revealing new insights into previously unknown formation processes.

Postdoctoral Fellow **University of Nebraska Lincoln**, 2016-2018

Graduate Research Assistant **University of Paris Est Marne La-Vallee**, 2013-2016

- Developed a new computational approach, combining multi- and mono-reference methods, enabling accurate description of the photochemistry of small negative anions.

TEACHING & MENTORING EXPERIENCE

Student Mentoring & Advising

- Undergraduate students
 - *Juliette Lipson* (University of Pennsylvania, Jan 2023-Jun 2023)
 - *Jacqueline Friskey* (University of Pennsylvania Jan 2022-Jun 2022)
 - *Natasa Rohacs* (University of Pennsylvania, Mar 2019-Dec 2019)
- Advised PhD thesis
 - *Vincent. J. Esposito* (University of Pennsylvania 2019-2022)
 - *Tongheng Chen* (University of Pennsylvania 2019-2020)
 - *Bilel Mehnen* (University of Tunis El-Manar 2016-2018)

Lecturer **University of Tunis El-Manar**, 2012- 2014

- Department of Physics
 - Taught “Mathematics for Physics” and “Introductory Physics”

Mentor & Tutor **Astronomical Society of Tunisia**, 2009-2016

- Provided mentorship and tutoring in astronomy-related activities and events.

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.

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, Icore-Pro, Molden, Gauss View, Gabedit)

- 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, modeling, 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)

- 79 T. **Trabelsi** & MF El-Tohamy, GAE, Mostafa and J.S. Francisco, Interstellar spectroscopic detection of HC(S)NC and DC(S)NC, [J. Chem. Phys.](#) 162,044307, (2025)
- 78 T. **Trabelsi** & J.S. Francisco, OCS₂ Isomers in the Venusian Atmospheric Chemistry: Spectroscopic Characterization and Photochemistry, [The Astrophysical Journal](#) 977,92, (2024)
- 77 T. **Trabelsi** & J.S. Francisco, Al₂O Photochemistry, [The Astrophysical Journal](#) 972,37(2024)
- 76 T. **Trabelsi**, J. Lipson and JS Francisco "ClSO and ClSO₂ Photochemistry: Implication for the Venusian Atmosphere" [J. Chem. Phys](#) 161,044303(2024)
- 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" [Chem. Eur. J](#) e202401397
- 73 J Xue, X Shao, J Li, J Li, T **Trabelsi**, J.S Francisco, X Zeng "Observation of the Water-HNSO₂ Complex" [J. Am. Chem. Soc.](#) 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](#) 146, 4162, (2024)
- 70 W. Chen, T. **Trabelsi**, X. Xu and J.S. Francisco "Spectroscopy of triatomic [Si,O,P] molecules" [Mol. Phys.](#) 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.](#) 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]” [Astron & Astrophys](#) 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 “HIO_x–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)

- 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 Vinoxyl and 1-Methylvinoxyl 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" [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 $[\text{Al},\text{N},\text{C},\text{O}]$ 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 AIOH the astrochemical reservoir molecule of AIO? 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 H^-+CO radiative association and HCO radiative electron attachment" [Faraday Discussion](#) [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)