Dr. Steve A. Ndengué

Contact Information

Visiting Assistant Professor
Department of Physics
Trinity College
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Hartford, CT 06106

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Computational Science Experience & Achievements

- Parallel Code Development, Multivariate Analysis, Numerical Modelling, Data Statistics.
- Developed a strong experience in analytical thinking, computer programming (Fortran, Bash, Python, Java, SQL, C++, Linux), problem solving and team management.
- Secured a $500K research grant to study photocatalysis and managed a team of 5 researchers.

Research Interests

Theoretical atomic and molecular physics: ab initio computations, reactive and non-reactive scattering, light-matter interaction, cold atoms, confined atoms and molecules, electric and magnetic response of atomic and molecular systems, fullerenes.
Theoretical physical chemistry: electronic structure, molecular spectroscopy, materials spectroscopy, astrochemistry, potential energy surfaces, classical and quantum dynamics, molecule-surface reactions, reaction rates, resonances, method development.

Academic Appointments

Visiting Assistant Professor July 2023 to Present
Department of Physics, Trinity College

Senior Lecturer (Hybrid) May 2019 to June 2023
ICTP-East African Institute of Fundamental Research, International Centre of Theoretical Physics (ICTP) and University of Rwanda (UR)

Postdoctoral Researcher November 2013 to April 2019
Department of Chemistry, Missouri University of Science and Technology

Lecturer & Senior Lecturer December 2011 to March 2015
Department of Physics, Faculty of Science, Université de Douala

Graduate Research Assistant October 2008 to December 2011
Laboratoire Interdisciplinaire de Physique, Université de Grenoble

Education

University of Grenoble, Grenoble, FRANCE

PhD, Condensed Matter and Radiation Physics, December 2011

- Thesis Topic: *Photodissociation of Ozone: Isotopic Selectivity*
- Advisors: Pr Rémy Jost, Pr Ousmanou Motapon, Dr Fabien Gatti
- Areas of Study: Molecular Physics, Physical Chemistry, Atmospheric Chemistry
- Funding: Agence Universitaire de la Francophonie (AUF) and Centre National de la Recherche Scientifique (CNRS).

University of Douala, Douala, CAMEROON

DEA (Master's Degree) with Honors, Particle and Radiation Physics, August 2007

- Adviser: Pr Ousmanou Motapon
- Area of Study: Atomic and Molecular Physics

Maîtrise (Bachelor's Honors) with Honors, Particle and Radiation Physics, September 2005

- Adviser: Pr Ousmanou Motapon
- Area of Study: Atomic and Molecular Physics

University of Buea, Buea, CAMEROON

Bachelor of Science with Honors, Physics, September 2003

- Major in Physics and Minor in Computer Science

Proposals

PI, "Embedded exact quantum dynamics for photocatalytic water splitting", Excellence in Africa – Junior Faculty Development Program, ICTP-EAIFR, 2021-2025 (Awarded): $767,000.
Co-PI: Nicola Marzari (EPFL).

Awards and Fellowships

- NSF & DOE Postdoctoral Research Funding, (2013–2019).
- ICTP-Simons Associate (Declined in favor of the NSF Fellowship), (2013–2016).
- Agence Universitaire de la Francophonie (AUF) Graduate Fellowship (2008–2011).
- Best student prize at the African School on Electronic Structure Methods and Applications (ASESMA 2008 and 2010).
- Travel grant for JAIST Winter School 2013 (Japan).
- Travel grant for RASESMA 2013 (Congo).
- Travel grant for ASESMA 2008 (South Africa), 2010 (South Africa) and 2012 (Kenya).

Book Chapters

[1] **Ndengué, S.A.**, and O. Motapon. Spatial and shell confinement of one electron atomic and molecular systems. In: K.D. Sen (Ed.), Chap. 7 *Electronic Structure of Quantum Confined Atoms and Molecules*. Springer (Switzerland), 2014.

Review Articles

[2] Dawes, R. and **S.A. Ndengué**. Single and Multireference Electronic Structure Considerations for ab initio based Potential Energy Surfaces. *International Reviews in Physical Chemistry*, 35(3):441. 2016.

Refereed Journal Publications

[3] Tajouo Tela, H., E.L. Quintas-Sanchez, M.-L. Dubernet, Y. Scribano, F. Gatti, R. Dawes and **S.A. Ndengué**. Rovibrational states of H_2O-HCN. *Physical Chemistry Chemical Physics*, In preparation. 2023.

[4] **Ndengué, S.**, E.L. Quintas-Sanchez, R. Dawes and D. Osborn. Temperature Dependence of the Electronic Absorption Spectrum of NO_2. *Journal of Physical Chemistry A*, Accepted, 2023.

[5] **Ndengué, S.**, E.L. Quintas-Sanchez, R. Dawes and D. Osborn. The low-lying electronic states of NO_2: potential energy and dipole surfaces, bound states, and UV absorption spectrum (Cover Article) *Journal of Physical Chemistry A*, 125(25):5519. 2021.

[6] Endres, E.S., **S. Ndengué**, O. Lakhmanskaya, S. Lee, F.A. Gianturco, R. Dawes and R. Wester OH^-+He temperature dependent inelastic collisions. *Physical Review A*, 103:052807. 2021.

[7] Bossion, D., **S. Ndengué**, H.D. Meyer, F. Gatti and Y. Scribano. Communication: Theoretical investigation of the H+HD→D+H_2 chemical reaction for astrophysical applications: a state-to-state quasi-classical study. *Journal of Chemical Physics*, 153:081102. 2020.

[8] Sur, S., **S.A. Ndengué**, E.L. Quintas Sanchez, C.T. Bop, F. Lique and R. Dawes. Rotationally inelastic scattering of O_3–Ar: State-to-state rates with the MultiConfigurational Time Dependent Hartree method. *Physical Chemistry Chemical Physics*, 22:1869. 2020.

[9] **Ndengué, S.A.**, Y. Scribano, F. Gatti and R. Dawes. State-to-state inelastic rotational cross sections in five-atom systems with the MCTDH method. *Journal of Chemical Physics*, 151:134301. 2019.

[10] Sur, S., E.L. Quintas Sanchez, **S.A. Ndengué** and R. Dawes. Development of a potential energy surface for the O_3–Ar system: Rovibrational states of the complex *Physical Chemistry Chemical Physics*, 21(18):9168. 2019.

[11] Han, S., X. Zheng, **S. Ndengué**, Y. Song, R. Dawes, D. Xie, J. Zhang and H. Guo. Dynamical Interference in the Vibronic Bond Breaking Reaction of HCO. *Science Advances*, 5:eaau0582. 2019.

[12] **Ndengué, S.A.**, Y. Scribano, D. Benoit, F. Gatti and R. Dawes. Intermolecular rovibrational bound states of H_2O-H_2 dimer from a MultiConfiguration Time Dependent Hartree approach. *Chemical Physics Letters*, 715:347. 2019.

[13] McCarthy, M.C., **S.A. Ndengué** and R. Dawes. The rotational spectrum and potential surface of the Ar-SiO complex. *Journal of Chemical Physics*, 149:134308. 2018.

[14] **Ndengué, S.A.**, R. Dawes, F. Gatti and H. Guo. Influence of the Renner-Teller coupling in the H+CO inelastic scattering. *Journal of Physical Chemistry A*, 122(31):6381. 2018.

[15] **Ndengué, S.A.**, R. Dawes, F. Gatti and H.-D. Meyer. Atom-Triatom Rigid Rotor Inelastic Scattering with the MultiConfiguration Time Dependent Hartree (MCTDH) approach. *Chemical Physics Letters*, 668:42. 2017.

[16] **Ndengué, S.A.**, R. Dawes and H. Guo. A new set of Potential Energy Surfaces for HCO: Influence of Renner-Teller coupling on the bound and resonance vibrational states. *Journal of Chemical Physics*, 144:244301. 2016.

[17] **Ndengué, S.**, R. Dawes, X.-G. Wang, T. Carrington, Z. Sun and H. Guo. Calculated Vibrational States of Ozone up to Dissociation. *Journal of Chemical Physics*, 144:074302. 2016.

[18] Majumder, M., **S.A. Ndengué**, and R. Dawes. Automated construction of potential energy surfaces. *Molecular Physics*, 114(1):1. 2016.

[19] Melingui Melono, R.L., A.J. Etindele, T. Tchakoua, **S.A. Ndengué** and O. Motapon. Polarizability of off-center spherically confined hydrogen atom. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 48:215001. 2015.

[20] Yu, H.-G., **S.A. Ndengué**, J. Li, R. Dawes, and H. Guo. Accurate vibrational energy levels of the simplest Criegee intermediate (CH_2OO) from full-dimensional quantum and MCTDH calculation. *Journal of Chemical Physics*, 143:084311. 2015.

[21] **Ndengué, S.A.**, R. Dawes, F. Gatti and H.-D. Meyer. Resonances of HCO computed using an approach based on the Multiconfiguration Time Dependent Hartree Method. *Journal of Physical Chemistry A*, 119(50):12043. 2015.

[22] **Ndengué, S.A.**, R. Dawes, and F. Gatti. Rotational Excitations in CO-CO Collisions at Low Temperature: Time Independent and Multiconfiguration Time Dependent Hartree Calculations. *Journal of Physical Chemistry A*, 119(28):7712. 2015.

[23] **Ndengué, S.A.**, S. Madronich, F. Gatti, H.-D. Meyer, O. Motapon, and R. Jost. Ozone photolysis: strong isotopologue/isotopomer selectivity in the stratosphere. *Journal of Geophysical Research: Atmosphere*. 119(7):4286. 2014.

[24] **Ndengué, S.A.**, O. Motapon, R.L. Melingui Melono, and A.J. Etindele. Electronic structure of cylindrically confined hydrogen atom by B-spline methods: Application to its dipole polarizability. *Journal of Physics B: Atomic, Molecular and Optical Physics*. 47:015002. 2014.

[25] **Ndengué, S.A.**, R. Schinke, F. Gatti, H.-D. Meyer, and R. Jost. Ozone Photodissociation: Isotopic and Electronic Branching Ratios for Symmetric and Asymmetric Isotopologues. *Journal of Physical Chemistry A*, 116(50):12271. 2012.

[26] **Ndengué, S.A.**, R. Schinke, F. Gatti, H.-D. Meyer, and R. Jost. Comparison of the Huggins band for six ozone isotopologues: vibrational levels and Absorption Cross Section. *Journal of Physical Chemistry A*, 116(50):12260. 2012.

[27] Motapon, O., **S.A. Ndengué**, and K.D. Sen. Static and dynamic dipole polarizablities and electron density at origin: Ground and excited states of hydrogen atom confined in multiwalled fullerenes. *International Journal of Quantum Chemistry*, 111(15):4425. 2011.

[28] **Ndengué, S.A.**, R. Schinke, F. Gatti, H.-D. Meyer, and R. Jost. Absorption cross-section of ozone isotopologues calculated with the Multiconfiguration Time-Dependent Hartree (MCTDH) method: I. The Hartley and Huggins bands. *Journal of Physical Chemistry A*, 114(36):9855. 2010.

[29] **Ndengué, S.A.**, and O. Motapon. Electron–electron interaction effects in heliumlike atoms confined in finite external square-well potential. *The European Physical Journal D-Atomic, Molecular, Optical and Plasma Physics*, 55(1):43. 2009.

[30] **Ndengué, S.A.**, and O. Motapon. Electric response of endohedrally confined hydrogen atoms. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 41:045001. 2008.

Conference Publications

[31] **Ndengué, S.A.**, R. Jost, F. Gatti, R. Schinke, H.-D. Meyer and O. Motapon. Absorption cross-section from Ab initio PESs and Wavepacket Propagation: the ozone test case. In: F. Tsobnang, C. Awono Onana, U. Chinje Melo (Eds.), *Formation, Recherche, Innovation et Développement Au Coeur de l'Interdisciplinarité, Actes des 3èmes Rencontres EG@ Yaoundé, Cameroun, 14-16 Septembre 2010*, L'Harmattan, March 2012.

Other Publications

[32] **Ndengué, S.A.** *Photodissociation of ozone molecule: isotopic selectivity.* PhD thesis, Université de Grenoble, Grenoble, France, 2012.

Invited Talks

[1] Ndengué, S.A.. Wavepacket studies of the water-dimer: Insights from exact quantum dynamics. In: *Lennard-Jones Centre Discussion Group - Cambridge Uni*, Online, October 2022. (Talk)

[2] Ndengué, S.A.. Wavepacket studies of the water-dimer: Insights from 12D quantum dynamics. In: *US-Africa Initiative on Electronic Structure Meeting*, Online, May 2022. (Talk)

[3] Ndengué, S.A.. Molecular Spectroscopy and Quantum Dynamics with Contracted and Optimized Basis: Applications in Atmospheric Physics and Astrochemistry. In: *Rutgers University-Newark, Department of Physics Seminar*, Newark, NJ, USA, October 2021. (Seminar)

[4] Ndengué, S.A.. The multiconfiguration time dependent Hartree (MCTDH) approach and applications in gas phase and condensed phase chemistry. In: *ICTP Atomistic Seminar*, Webinar, May 2020. (Seminar)

[5] Ndengué, S.A. Introduction to Hartree-Fock Method. In: *Regional African School on Electronic Structure Methods and Applications (RASESMA)*. Brazzaville, Congo, April 2013. (Lecture)

Conference Talks, Seminars, Posters and Abstracts

[6] Tajouo Tela, H., Y. Scribano, F. Gatti and S.A. Ndengué. The rigid rotor water-dimer with the MCTDH method: PES representation and rovibrational state calculations In: *Workshop on Machine Learning and Quantum Computing for Quantum Molecular Dynamics*, Marne-la-Vallée, France, September 2022. (Poster)

[7] Ndengué, S.A., M. Schröder, H.-D. Meyer, O. Vendrell, Z. Zhang, D.H. Zhang and F. Gatti Wavepacket studies of the water-dimer: Insights from 12D quantum dynamics. In: *Workshop on Machine Learning and Quantum Computing for Quantum Molecular Dynamics*, Marne-la-Vallée, France, September 2022. (Poster)

[8] Ndengué, S.A.. Wavepacket studies of the water-dimer: Insights from 12D quantum dynamics. In: *Psi-k Conference*, Lausanne, Switzerland, August 2022. (Poster)

[9] Ndengué, S.A.. Wavepacket studies of the water-dimer: Insights from 12D quantum dynamics. In: *Summer Theory Workshop on Molecules and Materials: Design and Dynamics (Rutgers University-Newark Physics Department)*, Newark, NJ, USA, June 2022. (Seminar)

[10] Ndengué, S.A.. Wavepacket studies of the water-dimer: Insights from 12D quantum dynamics. In: *2022 Workshop on Recent Developments in Electronic Structure (ES22)*, New-York, NY, USA, June 2022. (Talk)

[11] Ndengué, S.A., M.. Schröder and F. Gatti. Wavepacket simulation of the infrared spectrum of $(H_2O)_2$ in the OH-stretching region. In: *US-Africa Initiative on Electronic Structure Meeting*, Webinar, June 2021. (Talk)

[12] Ndengué, S.A., E.L. Quintas-Sanchez, F. Gatti, D. Osborn and R. Dawes. Elucidating the dynamics of complex gas phase molecular systems with MCTDH calculations. In: *African Physical Society International Conference*, Webinar, November 2020. (Talk)

[13] Ndengué, S.A., Y. Scribano, F. Gatti and R. Dawes. Benchmark Calculations of atom+triatom and diatom+triatom rigid rotor inelastic scattering with MCTDH In: *GDR THEMS*, Orsay, France, November 2019 (Talk)

[14] Ndengué, S.A. Time Independent and Dependent Ideas and Comparisons in Spectroscopy and Dynamics In: *Dynamics of Cold Molecular Collisions*, Orsay, France, November 2019. (Talk)

[15] Sur, S., S.A. Ndengué, E.L. Quintas-Sanchez and R. Dawes. Inelastic collision dynamics of O_3+Ar In: *International Symposium on Molecular Spectroscopy*, Champaign, IL, USA, June 2019. (Talk)

[16] Ndengué, S.A., R. Dawes, Y. Scribano and F. Gatti. MCTDH Computations of Inelastic Scattering and Molecular Spectroscopy for Astrochemically Relevant Molecules In: *ACS National Meeting*, Boston, MA, USA, August 2018. (Talk)

[17] Sur, S., E.L. Quintas-Sanchez, S.A. Ndengué and R. Dawes. Inelastic collisions of Ar and O_3 In: *International Symposium on Molecular Spectroscopy*, Champaign, IL, USA, June 2018. (Talk)

[18] Ndengué, S.A. and R. Dawes. MCTDH Rovibrational States and State-to-State Inelastic Scattering Calculations on the H_2O-H_2 System In: *International Symposium on Molecular Spectroscopy*, Champaign, IL, USA, June 2018. (Talk)

[19] Ndengué, S.A. Molecular Spectroscopy and Quantum Dynamics with Contracted and Optimized Basis. In: *Université Paris-Est Marne-La-Vallée, Laboratoire MSME*, Marne-La-Vallée, France, May 2018. (Seminar)

[20] Ndengué, S.A. Molecular Spectroscopy and Quantum Dynamics with Contracted and Optimized Basis. In: *Auburn University Physics Department Colloquium*, Auburn, AL, USA, March 2018. (Seminar)

[21] Ndengué, S.A. and R. Dawes. Some Applications of MCTDH to astrochemistry and combustion calculations. In: *Quantum Dynamics with the Multiconfiguration Time-Dependent Hartree (MCTDH) method: future and perspectives*, Orsay, France, October 2017. (Talk)

[22] Ndengué, S.A. and R. Dawes. Resonance and inelastic scattering calculations to understand the ozone isotopic anomaly. In: *3rd International Workshop: Spectroscopic and Dynamics of Ozone and Related Atmospheric Species*, Reims, France, October 2017. (Talk)

[23] Ndengué, S.A. and R. Dawes. Towards a quantum dynamical Study of the H_2O+H_2O inelastic collision: representation of the potential and preliminary results. In: *International Symposium on Molecular Spectroscopy 72nd Meeting.*, Champaign-Urbana, IL, USA, June 2017. (Talk)

[24] Ndengué, S.A. and R. Dawes. Influence of Renner-Teller coupling in the CO+H collisional dynamics. In: *International Symposium on Molecular Spectroscopy 72nd Meeting.*, Champaign-Urbana, IL, USA, June 2017. (Talk)

[25] Ndengué, S.A., R. Dawes and H. Guo. Electronically non-adiabatic effects in rovibrationally inelastic collisions. In: *Molecular Interactions & Dynamics Gordon Research Seminar and Gordon Research Conference*, Easton, MA, USA, July 2016. (Poster)

[26] Ndengué, S.A. and R. Dawes. Rovibrational Levels and Inelastic Scattering of the H_2O-Ar Cluster in Full and Reduced Dimensionality. In: *International Symposium on Molecular Spectroscopy 71st Meeting.*, Champaign-Urbana, IL, USA, June 2016. (Talk)

[27] Ndengué, S.A. and R. Dawes. Inelastic Scattering of H+CO: Influence of Renner-Teller Coupling. In: *International Symposium on Molecular Spectroscopy 71st Meeting. Session "Theory and Computation"*, Champaign-Urbana, IL, USA, June 2016. (Talk)

[28] Dawes, R., S.A. Ndengué, X.-G. Wang T. Carrington and H. Guo. Calculated Vibrational States of O_3 up to Dissociation. In: *International Symposium on Molecular Spectroscopy 71st Meeting. Minisymposium "Atmospheric Chemistry"*, Champaign-Urbana, IL, USA, June 2016. (Talk)

[29] Ndengué, S.A., R. Dawes and F. Gatti. Combined Time Dependent and Time Independent Study of Inelastic Scattering of the CO Dimer. In: *"Dynamics of Molecular Collisions 25th Meeting."*, Monterey, California, July 2015. (Poster)

[30] Ndengué, S.A.. Quantum Dynamics of Small and Medium Sized Molecules: Applications to Atmospheric Chemistry, Astrophysics, and Combustion. In: *"Department of Chemistry, Missouri University of Science and Technology"*, Rolla, Missouri, February 2015. (Seminar)

[31] Ndengué, S.A., R. Dawes, X.-G. Wang and T. Carrington. Some calculations with MCTDH: vibrational levels and resonances of small molecules. In: *"Chimie Théorique, Méthodologies et Modélisations"*, Montpellier, France, November 2014. (Seminar)

[32] Ndengué, S.A., R. Dawes, X.-G. Wang and T. Carrington. Some calculations with MCTDH: vibrational levels and resonances of small molecules. In: *"Groupe de Spectrométrie Moléculaire et Atmosphérique"*, Reims, France, November 2014. (Seminar)

[33] Ndengué, S.A., R. Dawes, X.-G. Wang and T. Carrington. Vibrational levels and resonances on a new potential energy surface for the ground state of ozone. In: *International Symposium on Molecular Spectroscopy 69th Meeting. Minisymposium "Spectroscopy in Kinetics and Dynamics"*, Champaign-Urbana, IL, USA, June 2014. (Talk)

[34] Etindele, A.J., S.A. Ndengué, R.L. Melingui Melono, T. Tchakoua, and O. Motapon. Investigation and Modelling of off-centre Endohedral Fullerenes. In: *7th Africa Materials Research Society Meeting*, Addis Ababa, Ethiopia, December 2013. (Abstract)

[35] Gatti, F., B. Lasorne, A. Perveaux, S. Ndengué, and R. Jost. Ozone photolysis: strong isotopologue/isotopomer selectivity in the stratosphere. In: *International Symposium on Molecular Spectroscopy 68th Meeting. Minisymposium "Spectroscopy of Planetary Atmospheres"*, Colombus, OH, USA, June 2013. (Abstract)

[36] Ndengué, S.A., A.J. Etindele, R.L.M. Melono, and O. Motapon. Investigation and modelling of endohedral fullerene: the atomic viewpoint. In: *Regional African School on Electronic Structure Methods and Applications (RASESMA)*, Brazzaville, Congo, April 2013. (Poster)

[37] Etindele, A.J., S.A. Ndengué, J.J. Fifen, and O. Motapon. Investigation and modelling of endohedral fullerene: the molecular viewpoint. In: *Regional African School on Electronic Structure Methods and Applications (RASESMA)*, Brazzaville, Congo, April 2013. (Poster)

[38] Etindele, A.J., S.A. Ndengué, J.J. Fifen, and O. Motapon. Modélisation de la structure des atomes confinés dans une cage de fullerène: Cas des atomes à un ou deux électrons de valence. In: *4th Euro Graduation Access Meeting*, Yaoundé, Cameroon, December 2012. (Poster)

[39] Ndengué, S.A., F. Gatti, H.-D. Meyer, R. Schinke, and R. Jost. The photodissociation isotope branching ratios of $^{16}O_3$, $^{17}O^{16}O_2$ and $^{18}O^{16}O_2$. In: *1st International Workshop: Spectroscopy and Dynamics of Ozone and Related Atmospheric Species*, Reims, France, October 2011. (Talk)

[40] Ndengué, S.A., F. Gatti, H.-D. Meyer, R. Schinke, and R. Jost. The Huggins eigenstates of $^{16}O_3$, $^{17}O^{16}O_2$ and $^{18}O^{16}O_2$. In: *Workshop on spectroscopy and dynamics of ozone and related atmospheric species*, Reims, France, October 2011. (Talk)

[41] Ndengué, S.A., F. Gatti, H.-D. Meyer, R. Schinke, and R. Jost. The Huggins eigenstates and the photodissociation branching ratio of $^{16}O_3$ and $^{18}O^{16}O_2$. In: *High Resolution Molecular Spectroscopy 2011 (HRMS2011)*, Dijon, France, August 2011. (Poster)

[42] Ndengué, S.A., A.J. Etindele, and O. Motapon. Cylindrically shell-confined one electron atoms: energy levels, electron localization and static dipole polarizability. In: *PCAM Summer School 2011*, San Sebastian, Spain, July 2011. (Poster)

[43] Ndengué, S.A., S. Madronich, R. Schinke, F. Gatti, H.-D. Meyer, and R. Jost. Isotope selectivity in atmospheric ozone photolysis. In: *European Research Course on Atmospheres (ERCA)*, Grenoble, France, January 2011. (Poster)

[44] Ndengué, S.A., R. Jost, F. Gatti, and R. Schinke. Ab initio absorption cross-section and photodissociation of ozone: photodissociation contribution to the ozone isotopic anomaly. In: *European Research Course on Atmosphere (ERCA)*, Grenoble, France, January 2011. (Poster)

[45] Ndengué, S.A., R. Jost, F. Gatti, R. Schinke, and O. Motapon. Absorption cross-section from ab initio potential energy surfaces and wavepacket propagation: the ozone test case. In: *3rd Euro Graduation Access Meeting*, Yaoundé, Cameroon, September 2010. (Talk)

[46] Ndengué, S.A., S. Madronich, R. Schinke, F. Gatti, H.-D. Meyer, and R. Jost. Isotope selectivity in atmospheric ozone photolysis. In: *European Geosciences Union Conference*, Vienna, Austrich, May 2010. (Poster)

[47] Ndengué, and O. Motapon. Finite basis investigation of confined atomic systems. In: *1st Cameroon Physical Society Conference*, Yaoundé, Cameroon, December 2009. (Abstract)

Research Visits

- August 2022: Laboratory of Theory and Simulation of Materials, Ecole Polytechnique Federale de Lausanne. *Host: Pr Nicola Marzari.*
- June 2022: Department of Physics, Rutgers University-Newark. *Host: Pr Neepa Maitra.*
- March 2017, November 2018: Institut de Sciences Moléculaires d'Orsay, Université Paris-Saclay. *Host: Pr Fabien Gatti.*
- March 2017, November 2018: Laboratoire Ondes et Milieux Complexes, Université du Havre. *Host: Dr Francois Lique.*
- November 2014: Groupe de Spectrométrie Moléculaire et Atmosphérique, Université de Reims Champagne-Ardennes. *Host: Pr Vladimir Tyuterev.*
- March 2009, February 2010, November 2014: Institut Charles Gerhardt, Université de Montpellier 2. *Host: Pr Fabien Gatti.*

Supervision

Postdoctoral Researchers

- **Ayda Badri**: Physics, University of Rwanda – ICTP-EAIFR. Embedded Exact Quantum Dynamics for Photocatalytic Water Splitting 2021–2022.

PhD Students

- **Wala Fathelrahman Ibrahim Elsayed**: Physics, University of Rwanda – ICTP-EAIFR. Ab-initio Insights into the Formation Mechanisms, Photocatalytic Activity, and Magnetic Properties of Magnetite/Silica/Titania Core-Shell Nanoparticles. co-advisers: Omololu Akin-Ojo (ICTP-EAIFR) and Nicola Seriani (ICTP). 2022–2025.
- **Sosthene Irambona**: Physics, University of Rwanda – ICTP-EAIFR. Embedded Exact Quantum Dynamics for Photocatalytic Water Splitting co-adviser: Omololu Akin-Ojo (EAIFR). 2021–2024.
- **Hervé Tajouo Tela**: Physics, University of Rwanda – ICTP-EAIFR. Spectroscopy and Dynamics of the Water-Dimer and other Water Clusters. co-adviser: Hassanali Ali (ICTP). 2020–2023.

MSc Students

- **Ange Benise Niyikiza**: Physics, University of Rwanda – ICTP-EAIFR. Quantum control of molecular processes: Towards quantum technologies in Chemistry. Co-adviser: Fabien Gatti (CNRS & Univ. Paris-Saclay). 2021–2022.
- **Jean Paul Nshuti**: Physics, University of Rwanda – ICTP-EAIFR. Quantum Dynamics in Condensed Phase: charge transfer in biological and organic photovoltaic systems. Co-adviser: Fabien Gatti (CNRS & Univ. Paris-Saclay). 2021–2022.

Mentoring

PhD Students

- **Sangeeta Sur**: Chemistry, Missouri S&T. Spectroscopy and Dynamics of the O_3-Ar cluster: Application to Ozone formation. Primary adviser: Richard Dawes. 2016–2019.
- **Anne Justine Etindele**: Physics, University of Douala. Electronic structure and polarizability of alkali atoms in fullerenes. Primary adviser: Ousmanou Motapon. 2011–2013.
- **Robert Landry Melingui Melono**: Physics, University of Douala. Polarizability of endohedrally confined small molecules using B-Splines. Primary adviser: Ousmanou Motapon. 2012–2013.

Maîtrise (Bachelor Honors) Students

- **Mabel Miyenga**: Physics, University of Douala. Energy levels and polarizability of confined alkali atoms with B-Splines. Primary adviser: Ousmanou Motapon. 2006–2007.
- **Alvine Kamaha**: Physics, University of Douala. Energy levels of the Helium atom using B-Splines. Primary adviser: Ousmanou Motapon. 2006–2007.
- **Chimene Daleu**: Physics, University of Douala. Relativistic energies of the Hydrogen atom using B-Splines. Primary adviser: Ousmanou Motapon. 2006–2007.
- **Roland Kamdem Mounchikpou**: Physics, University of Douala. Spatial confinement of hydrogen atom using the p-FEM. Primary adviser: Ousmanou Motapon. 2005–2006.

Teaching Experience

ICTP-East African Institute for Fundamental Research, Kigali, RWANDA

Lecturer **May 2019 to Present**

- Quantum Mechanics I
  - Fall 2021, 2022

- 1st year Master's students in Physics are introduced to basic concepts of quantum mechanics: one dimensional problems, Hermitean operators, harmonic oscillator, Heisenberg representation, angular momentum, spin.
- Responsible of 20 lectures and tutorials of 3 hrs each.

Lecturer **May 2019 to Present**

- Lecturer of Numerical Methods in Physics I
  - Fall 2019-2021, Spring 2022, 2023
  - 1st year Master's students in Physics are introduced to concepts on numerical methods in Physics such as root finding, linear algebra, numerical integration and differentiation, partial differential equations and coding in the Fortran language.
  - Responsible of 18 lectures and labs of 3 hrs each. Prepared the course material and tutorials and practicals.

Lecturer **May 2019 to Present**

- Lecturer of Numerical Methods in Physics II
  - Spring 2020
  - 2nd year Master's students in Physics are introduced to advanced concepts on numerical methods in Physics such as Monte Carlo methods, Molecular dynamics, numerical differential equations and coding in the Fortran and Python languages.
  - Responsible of 18 lectures and labs of 3 hrs each. Prepared the course material and tutorials and practicals.

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Lecturer **May 2013 to November 2013**

- Lecturer of IN 170: Undergraduate Course in Algorithmics
  - Fall 2013
  - 1st year students in Physics and Chemistry were introduced to basic concepts in computer science and algorithmics based on Python programming language.
  - Responsible of 4-hours lecture weekly. Prepared the course material and tutorials.
- Lecturer of PH 520: Graduate Course on Numerical Methods in Physics
  - Spring 2013
  - Graduate students in Physics worked on methods to solve differential equations relevant to physics problems using Fortran and Matlab programming language.
  - Responsible of 2-hours lecture weekly. Prepared the course material and practicals.

Teaching Assistant **December 2011 to July 2013**

- Instructor of PH 422: Graduate Course in Atomic Physics
  - Fall 2011 and 2012
  - Graduate students in Physics applied quantum mechanics principles to various problems in atomic physics such as understanding their structure and their interaction with electromagnetic field.
  - Responsible of 2-hours tutorials weekly. Prepared the course tutorials. Provided and graded the exams.
- Instructor of PH 428: Graduate Course in Numerical Analysis
  - Fall 2012
  - Graduate students in Physics worked on methods to solve differential equations relevant to physics problems using Fortran and Matlab programming language.
  - Responsible of 4-hours tutorials and practical weekly. Prepared the course tutorial and practicals. Provided and graded the exams.
- Instructor of PH 120/121: Undergraduate Course on Evolution Laws in Physics
  - Autumn 2012 and Winter 2012
  - 1st year Physics, Chemistry and Mathematics students are introduced to the modelisation of physical systems and analytic resolution of 1st and 2nd order differential equations resolving from the models.
  - Responsible of 4-hours tutorials and practical weekly. Graded the exams.

- Instructor of PH 142: Undergraduate Course in Mechanics and Spatial Dynamics
  - Spring 2012 and 2013
  - 1st year students in Physics and Mathematics are introduced to solid mechanics and spatial dynamics.
  - Responsible of 6-hours tutorials weekly. Provided and graded the exams.
- Instructor of IN 131: Undergraduate Course in Computer Science
  - Fall 2012
  - 1st year students in Physics and Mathematics are introduced to computer science and automatic treatment of information.
  - Responsible of 4-hours tutorials and practical weekly. Graded the exams.

Professional Service

Conference Organisation

- Member of the organizing comittee with Omololu Akin-Ojo (ICTP-EAIFR), G. Gebreyesus Hagoss (University of Ghana), Sinead Griffin (LBNL), Richard Martin (Stanford University), Shobhana Narasimhan (JNCASR Bangalore) and Nicola Seriani (ICTP)
  7th African School on Electronic Structure Methods and Applications (ASESMA), June 2023, Kigali, Rwanda.
- Member of the organizing comittee with Omololu Akin-Ojo (ICTP-EAIFR), G. Gebreyesus Hagoss (University of Ghana), Sinead Griffin (LBNL), Richard Martin (Stanford University), Shobhana Narasimhan (JNCASR Bangalore) and Nicola Seriani (ICTP)
  African School on Electronic Structure Methods and Applications (ASESMA), June 2021, Online.
- Co-organizer with Omololu Akin-Ojo (ICTP-EAIFR), Douglas Buttrey (University of Delaware)
  African School of Catalysis 2020, January 2020, Kigali, Rwanda.
- Co-organizer with Omololu Akin-Ojo (ICTP-EAIFR), Gian-Marco Rignanese (Université Libre de Bruxelles) and Phillipe Ghosez (Université Libre de Bruxelles)
  Regional African School on Electronic Structure Methods and Applications (RASESMA) with Abinit, January 2020, Kigali, Rwanda.

Associate Editor Service

- *African Physics Newsletter*

Referee Service

- *Applied Surface Science*
- *Chemical Physics Letters*
- *Journal of Physical Chemistry A*

Conference Service

- Chair of Session: *Electronic Structure, Potential Energy Surfaces*.
  International Symposium on Molecular Spectroscopy 2018, Champaign, IL, June 2018.
- Chair of Session: *From Potential Energy Surfaces to Dynamics and Kinetics*.
  256th ACS National Meeting, Boston, MA, August 2018.

Professional Experience

Missouri University of Science and Technology, Rolla, MO

Postdoctoral Researcher — **November 2013 to April 2019**

- Supervisor: Dr Richard Dawes
- Funding: National Science Foundation (NSF) & Department of Energy (DOE) :
  Molecular Dynamics on Multiple Potential Energy Surfaces.
  - Calculations of positions and lifetimes of bound and resonant states of molecules of atmospheric and combustion interest.
  - Non reactive molecular scattering for astrochemistry and combustion interest.
  - Numerical methods for nuclear quantum dynamics.

Université de Douala, Douala, Cameroon

Senior Lecturer — **December 2013 to March 2015**

Lecturer — **December 2011 to December 2013**

- Teaching graduate and undergraduate courses in Physics.
- Research in atomic and molecular physics.
  - Photodissociation of triatomic molecules.
  - Electronic structure and response of confined atomic and molecular systems.

NGO APICA, Douala, Cameroon

Consultant **February 2004 to July 2004**

- Monitoring projects and actions of local groups funded by a Mondial Bank program (Programme de Développement Participatif Urbain Fourmi II).

Professional Memberships and Associations

- American Physical Society, Member, 2015–Present
- American Chemical Society, Member, 2018–Present
- Réseau Confluens des anciens boursiers AUF, Member, 2015–Present
- Cameroon Physical Society, Member, 2010–Present
- Société Francaise de Physique, Junior member, 2010–2011

Application Areas

Chemical reaction dynamics, Confined atomic and molecular systems, Atmospheric chemistry, Astrochemistry, Astrophysics, Combustion, Catalysis, Biophysics.

Software Skills

Computer Programming:
- Fortran, C, C++, Pascal, Java, Julia, Python, Octave/Matlab, R
- OpenMP, MPI, Git, UNIX shell scripting, GNU make

Codes:
- User: MCTDH, Quantics, MolScat, Hibridon, Quantum Espresso, Gaussian

Numerical Analysis:
- Python, Octave/Matlab

Desktop Editing and Productivity Software:
- Vim, Emacs
- TEX(LATEX, BIBTEX)
- Microsoft Office, OpenOffice, LibreOffice
- GIMP

Operating Systems:
- Microsoft Windows family, Linux, Mac OS X

References Available to Contact

Prof. Richard Dawes (e-mail: dawesr@mst.edu; phone: +1-573-341-4451)
- Program Director National Science Foundation
- Adjunct Professor Department of Chemistry
  Missouri University of Science and Technology
  - ◇ 2415 Eisenhower Ave Alexandria, VA 22314
  - ⋆ *Dr. Dawes was my postdoctoral supervisor.*

Prof. Fabien Gatti (e-mail: fabien.gatti@universite-paris-saclay.fr; phone: +33-1-6915-8283)
- Research Professor, Institut des Sciences Moléculaires d'Orsay
  Centre National de la Recherche Scientifique
  - ◇ Institut des Sciences Moléculaires d'Orsay, UMR 8214 Bâtiment 210
    Université Paris-Sud 91405 Orsay Cedex, France.
  - ⋆ *Prof. Gatti is a former adviser, a mentor and a collaborator.*

Dr. Yohann Scribano (e-mail: yohann.scribano@umontpellier.fr; phone: +33-4-6714-4535)
- Associate Professor, Laboratoire Univers et Particules de Montpellier
  Université de Montpellier
  - ◇ LUPM UMR 5299, Université de Montpellier - Campus Triolet
  - ◇ Place Eugène Bataillon - CC 72 – 34095, Montpellier Cédex 05, France.
  - ⋆ *Dr. Scribano is a collaborator.*

More Information

- Google Scholar Profile
- ResearchGate Profile
- Orcid Profile
- Web of Science Profile