

Steve Ndengué

Curriculum Vitae

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Research Interests

- Atomic and electronic structure, ab initio computations, confined atoms and molecules, cold atoms,
Molecular reactive and non-reactive scattering, electric and magnetic response of atomic and
physics molecular systems, laser-matter interaction, fullerenes.
Theoretical spectroscopy, astrochemistry, potential energy surfaces, classical and quantum dynamics,
and physical scattering cross-sections, reaction rates, resonances.
chemistry

Experience

Teaching-Research

- 11/2013– Present **Postdoctoral Research Fellow**, Missouri university of Science and Technology, Rolla, Missouri.
"Spectroscopy and Dynamics of small molecules" in Richard Dawes Group in the Chemistry Department
- 12/2011– **Lecturer/Senior Lecturer**, Université de Douala, Douala, Cameroon.
- 03/2015 Teaching and Research in the Physics Department.
- Teaching: Atomic Physics, Numerical Analysis, General Physics, Quantum Physics, Classical Mechanics, Algorithmics
 - Research: Chemical Reaction Dynamics, Confinement of atoms and molecules

Humanitarian

- 02/2004– 06/2004 **Consultant**, NGO APICA (*Association pour la Promotion des Initiatives Communautaires Africaines*), Douala, Cameroon.
Monitoring projects and actions of local groups funded by a Mondial Bank program (Programme de Développement Participatif Urbain Fourmi II).

Education

- 2008–2011 **PhD Thesis in Physics**, Université de Grenoble, Grenoble, France.
 - Title: Photodissociation of Ozone: Isotopic Selectivity (in French)
 - Advisors: Pr Rémy Jost, Pr Ousmanou Motapon and Pr Fabien Gatti
 - Area of Study: Molecular Physics, Chemical Physics, Atmospheric Chemistry
- 2005–2007 **Diplôme d'Études Approfondies (DEA) en Physique**, Université de Douala, Douala, Cameroun, *Mention Bien*.
Area of Study: Atomic and Molecular Physics

2004–2005 **Maîtrise de Physique**, *Université de Douala*, Douala, Cameroun, *Mention Bien*.

Area of Study: Atomic and Molecular Physics

2000–2003 **BSc. in Physics**, *University of Buea*, Buea, Cameroun, *GPA – 3.16/4*.

Minor: Computer Science

Grants, Awards and Fellowships

2013-2018 ICTP-Simons Associate (Declined in Favor of Postdoctoral Fellowship)

2008-2011 Agence universitaire de la Francophonie (AUF) Graduate Fellowship

2008,2010 Best Student prize at the African School on Electronic Structure Methods and Applications (ASESMA 2008 and 2010)

Scientific Publications & Communications

Thesis

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

Book Chapter

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.

Refereed Journal Publications

1. 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*, In press. 2015.
2. 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.
3. 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*, In press. 2015.
4. 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.
5. 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.
6. 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.

7. 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.
8. 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.
9. Motapon, O., S.A. Ndengué, and K.D. Sen. Static and dynamic dipole polarizabilities 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.
10. 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.
11. 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.
12. 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 Publication

1. 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 EGØ Yaoundé, Cameroun, 14-16 Septembre 2010*, L'Harmattan, March 2012

Conference and Seminars Talks, Posters and Abstracts

1. 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, CA, USA, July 2015. (Poster)
2. 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. (Talk)
3. 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. (Talk)

4. 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. (Talk)
5. 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)
6. 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)
7. 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"*, Columbus, OH, USA, June 2013. (Contribution)
8. 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)
9. Ndengué, S.A. Introduction to *Ab initio* Methods. In: *Regional African School on Electronic Structure Methods and Applications (RASESMA)*. Brazzaville, Congo, April 2013. (Invited Talk)
10. 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. (Contribution)
11. 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. (Contribution).
12. Ndengué, S.A., F. Gatti, H.-D. Meyer, R. Schinke, and R. Jost. The photodissociation isotope branching ratios of $^{16}\text{O}_3$, $^{17}\text{O}^{16}\text{O}_2$ and $^{18}\text{O}^{16}\text{O}_2$. In: *Workshop on spectroscopy and dynamics of ozone and related atmospheric species*, Reims, France, October 2011. (Contribution)
13. Ndengué, S.A., F. Gatti, H.-D. Meyer, R. Schinke, and R. Jost. The Huggins eigenstates of $^{16}\text{O}_3$, $^{17}\text{O}^{16}\text{O}_2$ and $^{18}\text{O}^{16}\text{O}_2$. In: *Workshop on spectroscopy and dynamics of ozone and related atmospheric species*, Reims, France, October 2011. (Talk)
14. Ndengué, S.A., F. Gatti, H.-D. Meyer, R. Schinke, and R. Jost. The Huggins eigenstates and the photodissociation branching ratio of $^{16}\text{O}_3$ and $^{18}\text{O}^{16}\text{O}_2$. In: *High Resolution Molecular Spectroscopy 2011 (HRMS2011)*, Dijon, France, August 2011. (Poster)

15. 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)
16. 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)
17. 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)
18. 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)
19. 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, Austria, May 2010. (Contribution)
20. Ndengué, and O. Motapon. Finite basis investigation of confined atomic systems. In: *1st Cameroon Physical Society Conference*, Yaoundé, Cameroon, December 2009. (Contribution)

Professional Service

Reviewer: Chemical Physics Letters

Professional Memberships and Associations

American Physical Society, Member, 2015–Present

Réseau Confluens des anciens boursiers AUF, Member, 2015–Present

Cameroon Physical Society, Member, 2010–Present

Société Francaise de Physique, Junior Member, 2010–2011

Software Skills

Computer Programming C, C++, Fortran, Pascal, Python, Java, OpenMP, UNIX shell scripting, GNU make

Codes MCTDH, Quantum Espresso, Gaussian, MOLSCAT

Numerical Analysis Python, MATLAB

Editing and Productivity Vim, Emacs, T_EX(L_AT_EX,BI_BT_EX), MS Office, Open Office, Libre Office, iWork, GIMP

Operating Systems MS Windows Family, Linux, Mac OS X

■ Languages

French **Fluent**

Native

English **Excellent**

Speaking, reading and writing

■ Interests

Sport Basketball, Soccer, Hiking

Others Reading, auteur theory, travel, internet, IT

Computer Science Coding, Open Source

■ References

Available upon request.