Jacob Fosso Tande, Ph.D

Education

Doctorate of Philosophy in Physical Chemistry December 2012
The University of Tennessee/Oak Ridge National Laboratory in Knoxville, Tennessee, USA
Thesis Topic: Confinement Effects of Solvation on a Molecule Physisorbed on a Metal Particle.
- Advisor: Professor and Director of IACS, Stony Brook University, Robert J. Harrison.
- Concentration: Theoretical and Computational Chemistry.
- Minor: Interdisciplinary Graduate Minor in Computational Science.

Masters of Science in Chemistry August 2007
East Tennessee State University, Johnson City, Tennessee USA
- Thesis Topic: A Computational Chemistry Study of Spin Traps.
- Advisor: Dr. Scott J. Kirkby.
- Concentration: Physical Chemistry.

Bachelor of Science in Chemistry July 2002
University of Buea (UB), Buea, Southwest region, Republic of Cameroon.
- Professional Minor in Chemical Process Technology.

Research Interests

- Visualization on HPC systems: I am interested in understanding how visualization applications, network performance and computer resources can be put together to give the end-user an efficient, consistent and reliable visualization experience.

- Quality control for a better end-user experience
- Collaborative and reproducibility software and applications environment

HPC Experience

- Colby College's Research and Teaching Cluster   2017-Present
- University of New England Research group HPC   2016 – 2017
- Florida State Universty HPC   2014- 2016
- NERSC's Hopper on Cray XE 6   2013- 2014

- Kraken XT5 Cray system and University of Tennessee's HPC   2009- 2014

- Jaguar XT3 and XT4, Lens visualization cluster and TITAN at ORNL   2007- 2012

Professional Experience

Scientific Computing Coordinator, Colby College, Waterville Maine USA July 2017 – Present
Research Associate   May 2016- July 2017
University of New England, Portland, Maine, USA
Post-Doctoral Researcher   April 2014- May 2016
The Florida State University, Tallahassee, Florida, USA
Post-Doctoral Research Associate   January 2013- March 2014
The University of Tennessee, Knoxville, Tennessee, USA
Graduate Research Assistant   August 2007- December 2012
The University of Tennessee/Oak Ridge National Laboratory in Knoxville, Tennessee.
Graduate Research Assistant   September 2005- August 2007
East Tennessee State University in Johnson City, Tennessee

Teaching Experience

Adjunct Faculty, Central Maine Community College, Auburn Maine USA.
Intermediate Algebra.   Spring 2018 – Present
Assistant Instructor, University of New England, Portland Maine USA .
Introduction to Unix Computing and Molecular Visualization.   Winter 2017
Adjunct Faculty, Central Maine Community College, Auburn Maine USA.
Intermediate Algebra.   Spring 2017
Business Mathematics.   Spring 2017
Adjunct Faculty, Southern Maine Community College, South Portland Maine USA.
College Algebra.   Fall 2016
The University of Tennessee, Knoxville Tennessee USA.
Head Teaching Assistant General Chemistry.   Spring 2009
Teaching Assistant for CHEM240 (Chemical Programming).   Fall 2008 and Fall 2009
Web Master for General Chemistry.   Fall 2007
Laboratory Instructor for General Chemistry.   Fall 2007
East Tennessee State University, Johnson City Tennessee USA.
Upward Bound Program, physics and chemistry instructor .   May -- August 2007
Laboratory Instructor for General and Organic Chemistry.   2005-2007
Martin-Luther King Bilingual High School, Republic of Cameroon.
Physical Sciences and Mathematics Instructor.   August 2002 to September 2005
Discipline Master.   *August 2002 to September 2005*

Student Researchers Mentored

- Brandon Troisi. Summer intern. Received training on fundamental Linux command, Linux, Mac OS X operating systems, basic concepts on verification and validation of applications for download. Standard procedure of software installation and classroom computer imaging. Summer 2018
- Jessica White and Katie Chalmers. REU NSF Fellowship recipients. Developed coarse-grained

models for simulation of membrane-cation binding, Summer 2017, UNE Portland ME.
- Cody Black, NSF REU Fellow (2016). Studied mechanism of lipopolysaccharide (endotoxin) transport by MsbA; independent study student (2017); 2017 American Foundation for Pharmaceutical Education Gateway to Research Award.
- Rachel McDevitt. 2016 Summer REU NSF Fellow. Studied cholesterol recognition motifs in Pglycoprotein; judged the Protein Modeling event at the Maine Science Olympiad for high school students.

Peer-Reviewed Publications

- **Jacob Fosso-Tande** ,Cody Black, Stephen G. Aller, Lanyuan Lu, and, Ronald D. Hills Jr. AIMS Molecular Science, 4 (3):352-369 (2017) "Simulation of lipid-protein interactions with the CgProt force field."

- **J. Fosso-Tande** , T.-S. Nguyen, G. Gidofalvi, and A. E. DePrince III, J. Chem. Theory Comput., (2016). "Large-scale v2RDM-driven CASSCF method http://dx.doi.org/10.1021/acs.jctc.6b00190.

- Robert J. Harrison, Gregory Beylkin, Florian A. Bischoff, Justus A. Calvin, George I. Fann , **Jacob Fosso-Tande**, Diego Galindo , Jeff R. Hammond , Rebecca Hartman-Baker , Judith C. Hill , Jun Jia , Jakob S. Kottmann, M-J. Yvonne OU, Laura E. Ratcliff, Mathew G. Reuter, Adam C. Richie-Halford , Nichols A. Romero, Hideo Sekino, William A. Shelton, Bryan E. Sundal, W. Scott Thornton , Edward F. Valeev, Alvaro Vazquez-Mayagoitia, Nicholas Vence, and Yukina Yokoi. "MADNESS: A Multiresolution, ADaptive Numerical Environment for Scientific Simulation" , SIAM Journal on Scientific Computing, (2015) http://epubs.siam.org/doi/10.1137/15M1026171

- **Jacob Fosso-Tande** , Daniel R. Nascimento and A. Eugene DePrince III, Accuracy of two-particle N-representability condition for describing different spin states and the singlet-triplet gap in linear acene series, Molecular Physics, 114 (3-4), 423-430, (2015), http://dx.doi.org/10.1080/00268976.2015.1078008

- **J. Fosso-Tande** , R. J. Harrison. Confinement effects of solvation on a molecule physisorbed on a polarizable continuum particle Comput. Theo. Chem. 1017, 22-30 (2013), https://doi.org/10.1016/j.comptc.2013.05.006

- O. Gunaydin-Sen, P. Chen, **J. Fosso-Tande** , J. L. White, T. L. Allen, J. Cherian, and T. Tokumoto, P.M. Lahti, S.McGill, R. J. Harrison, and J. L.Musfeldt. Magnetoelectric coupling in 4,4'-stilbenedinitrene J. Chem. Phys., 138,204716 (2013), http://dx.doi.org/10.1063/1.4807053

- **J. Fosso-Tande** , R. J. Harrison. Implicit solvation models with multiresolution multiwavelet basis function. Chemical Physics Letters, 561–562, (2013) 179–184

- O. Gunaydin-Sen, **J. Fosso-Tande**, P. Chen, J. L. White, T. L. Allen, J. Cherian, and T. Tokumoto, P. M. Lahti, S. McGill, R. J. Harrison, and J. L. Musfeldt. Manipulating

the singlet-triplet equilibrium in organic biradical materials J. Chem. Phys., 135, 241101 (2011) http://dx.doi.org/10.1063/1.3672101

Invited Talks and Poster Presentation

- Ronald D. Hills Jr., **Jacob Fosso Tande,** Cody Black**,** Model Assessment and Simulation of Lipid-Protein Interactions, Biophysical Journal, Volume 112, Issue 3, Supplement 1, p528a, 3 February 2017

- Cody Black , **Jacob Fosso Tande,** Rachel McDavitt, and Ronald D. Hills Jr., LPS and Substrate Binding by Multidrug Efflux Proteins ,College of Pharmacy, University of New England, Portland, ME, Annual student research symposium., December 2016

- **Jacob Fosso-Tande** and A. Eugene Deprince III, "Large active-space-based calculations with variational 2-electron reduced density method", SETCA 2015, University of Central Florida, Orlando Fl, May 14-16, poster number 10, *poster presentation*

- **Jacob Fosso-Tande** "overcoming the challenge of accuracy in the analysis of the electronic structure of molecules", Department of Chemistry and Forensic Science, Savannah State University, Savannah Ga, May 1st 2015. *oral presentation*

- **Jacob Fosso-Tande,** Ozge Gunaydin-Sen, Peng Chen, Paul M Lahti, Janice L Musfeldt, Robert J Harrison. "Investigating the absorption features and biradical character in open-shell organic compounds.", 247th American Chemical Society National Meeting and Exposition of March 16-20, (2014), in Dallas, Texas, poster number 211. *poster presentation*

- J. L. Musfeldt , O. Gunaydin-Sen , P. Chen , **J. Fosso-Tande** , T. Allen , J. Cherian , T. Tokumoto , S. McGill , P.M. Lahti ,and R.J. Harrison. "Magnetoelectric coupling in 4, 4'-stilbenedinitrene.", APS March Meeting Abstract ID: BAPS.2013.MAR.C16.12 (2013) *oral presentation*

- **Jacob Fosso-Tande,** Ariana Beste, Robert J. Harrison. "Investigating the tunability of singlet-triplet equilibrium in organic biradical compounds", Gordon Research   Conference   on Computational Chemistry, Mount Snow Resort, West Dover, Vertmont   July   22-27   (2012) *poster presentation*

- **Jacob Fosso-Tande**   "Confinement effects of solvation on a molecule physisorbed on a polarizable continuum particle*.", i*nvited guess speaker, Argonne Leadership Computing Facility in Argonne, Illinois. December 17th 2012. *oral presentation*

- **Jacob Fosso-Tande** "Confinement effects of solvation on a molecule physisorbed on a metal particle." SETCA, Athens, Georgia May 17-19 (2012) *poster presentation*

- **Jacob Fosso-Tande**, Robert J. Harrison. "Implicit solvation model with multiresolution multiwavelet basis function.", 243rd ACS March Meeting in San Diego, California, publication number 581 March 25-29 (2012) *Oral Presentation*

- O. Gunaydin-Sen, **J. Fosso-Tande**, P. Chen, J. L. White, T. L. Allen, J. Cherian, and T. Tokumoto, P. M. Lahti, S. McGill, R. J. Harrison, and J. L. Musfeldt. "Manipulating the singlet-triplet equilibrium in organic biradical materials.", APS March Meeting Volume 56, Number 1 (2011) *oral presentation*

- **J. Fosso-Tande**, Compton, R., R. J. Harrison. "Modeling the charge transfer distribution in Buckminster Fullerene.", May (2008) SETCA conference, University of Alabama,Tuscaloosa Alabama, USA**,** poster number 24, *poster presentation*

- **J. Fosso-Tande**, Scott J. Kirkby, "A Computational Chemistry Study of Phenyl-N-Ter-Butyl Nitrone Spin Traps", 59th Southeastern Regional Section of the American Chemical Society of October 24 -27, 2007, in Green Ville, South Carolina, publication number 432 _oral presentation_
- **J. Fosso-Tande**, Scott J. Kirkby. "A Computational Chemistry Study of Spin-trap Molecules.", publication number 28, Spring (2007) Appalachian Student Research Forum, Johnson City, Tennessee USA. J. Fosso-Tande, Scott J. Kirkby. A Computational Chemistry Study of Spin-trap. _poster presentation_
- **J. Fosso-Tande**, Scott J. Kirkby. "A Computational Chemistry Study of Spin-trap Molecules.", 58th Southeastern Regional Section of the American Chemical Society of November 1st -4th, 2006, in Augusta, Georgia . _poster presentation_