

Curriculum Vitae

Adeayo O. Ajala, Graduate Assistant
Department of Chemistry, Michigan State University
Chemistry Building, 578 S. Shaw Lane, Room 18A
East Lansing, Michigan 48824-1322, USA
Current Mailing Address: 1821 W. Grand River Ave, Apt H1, Okemos, Michigan 48864
Telephone: (517)353-1154; (615)582-1101 (mobile)
Email: ajalaade@chemistry.msu.edu

Education

August 2012 – present, pursuing Ph.D. in theoretical and computational chemistry at Michigan State University. Advisor: Professor Piotr Piecuch
M.S., 2012, Chemistry, Tennessee State University, Nashville, Tennessee. Concentration: Organic Chemistry and Modeling
B.S., 2007, Chemistry, Obafemi Awolowo University, Ile-Ife, Nigeria
Minor, 2007, Physics, Obafemi Awolowo University, Ile-Ife, Nigeria

Research Experience

Graduate student researcher, August 2012 – present, Michigan State University. Advisor: Professor Piotr Piecuch.

I have benchmarked a variety of the equation-of-motion coupled cluster (EOMCC) theories, with a focus on the completely renormalized (CR) triples corrections to EOMCCSD energies, using a database of 28 small to medium-sized organic molecules including aliphatic hydrocarbons, aromatics and heterocycles, aldehydes and ketones, amides, and nucleobases, and about 150 excited states total. The main goal of this project has been to test the performance of the size intensive δ -CR-EOMCC methods against the established theoretical approximations, such as CASPT2, linear response CC3, and EOMCCSDT-3, and the available experimental data. The results obtained have been evaluated statistically and the outcomes have been compared with those available in the literature. We plan to extend this study to other EOMCC schemes.

My work has also included the application of the coupled-cluster active-space idea to the development of new-variants of the doubly electron-attached equation-of-motion coupled-cluster methods with up to 4-particle-2-hole ($4p$ - $2h$) excitations, resulting in a much more cost-effective model at the active-space $3p$ - $1h$ level.

Graduate student researcher, August 2010 – July 2012, Tennessee State University. Advisor: Professor Cosmas Okoro.

I examined 3D quantitative structure-activity relationships (QSAR) on 17 fluorinated hexahydropyrimidine, acridone derivatives, and determined their biological activities using Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Field Analysis (CoMSIA). Both models predict higher activities, better potency, and selectivity for some novel compounds obtained by structural modification of existing ones. Those compounds have been synthesized and test confirming our theoretical predictions made.

Sales Representative and Business Development Officer, December 2009 – April 2010, Q-Med Diagnostics and Ajayi's Travisil, Nigeria.

I was employed to market Travisil products, a pharmaceutical company based in India, in Lagos, Nigeria metropolitan cities. I wrote proposals on behalf of Q-Med and helped market their services among corporate outfits in Lagos.

High School tutor, October 2008 – September 2009, National Youth Service Corps, Nigeria.

I taught chemistry at Dority International School as part of my mandatory one-year service to the Nigerian nation.

Undergraduate student researcher, 2006-2007, Obafemi Awolowo University, Nigeria.

I worked with Professor Jide Ige. I performed an efficient statistical thermodynamics calculation of some simple cyclic organic compounds by determining their heat capacities.

Professional Experience

Michigan State University, August 2012 - present, Graduate Teaching and Research Assistant. Teaching freshman and junior levels chemistry as well as performing Ph.D. research in theoretical and computational chemistry. Ph.D. Advisor: Professor Piotr Piecuch.

Publications

Adeayo O. Ajala and Cosmas O. Okoro, "CoMFA and CoMSIA Studies on Fluorinated Hexahydropyrimidine Derivatives," *Bioorg. Med. Chem. Lett.* **21**, 7392 (2011).

Adeayo O. Ajala and Cosmas O. Okoro, "3D-QSAR Topomer CoMFA Studies on N-Substituted Acridone Derivatives," *Open Journal of Medicinal Chemistry* **2**, 43 (2012).

P. Piecuch, J.A. Hansen, and A.O. Ajala, "Benchmarking the Completely Renormalized Equation-of-Motion Coupled-Cluster Approaches for Vertical Excitation Energies," *Mol. Phys.*, **113**, 3085-3127 (2015) [Special Issue in Honor of Professor Sourav Pal; invited contribution, in response to an invitation issued to P. Piecuch].

A.O. Ajala, J. Shen, and P. Piecuch, "Development and Testing of New-Variants of Active-Space Doubly Electron-Attached Equation-of-Motion Coupled-Cluster Methods," in preparation

Talks Presented by Co-Authors

J.A. Hansen, N.P. Bauman, A.O. Ajala, B.G. Levine, M. Ehara, and P. Piecuch, "Development and Application of Numerical Methods for the Determination of Molecular Properties of Ground and Excited States Using Coupled-Cluster Approaches," Quantum Chemistry Research Institute, Kyoto, Japan, May 9, 2014.

J.A. Hansen, N.P. Bauman, A.O. Ajala, B.G. Levine, M. Ehara, and P. Piecuch, "Catalytic and Excited State Properties using Highly Correlated Electronic Structure Methods," Institute for Molecular Science, Okazaki, Japan, April 14, 2014.

Poster Presentation Given by Adeayo O. Ajala

A.O. Ajala, J.A. Hansen, and P. Piecuch, "Benchmarking the Renormalized Equation-of-Motion Coupled-Cluster Approaches for Vertical Excitation Energies", Midwest Theoretical Chemistry Conference, Ann Arbor, Michigan, USA, June 26-28, 2015

Fellowship

I was one of the 32 graduate students' fellows selected among various research groups in the U.S. to attend the Second Annual Software-Development Summer school for Computational Chemistry and Materials Modeling held at Stony Brook University in Stony Brook, NY, July 8-18, 2014.

Awards

Professor Layi Ogunkoya Prize for the best graduating student in Chemistry with the highest score not less than 60-B in CHM 307 (Application of Spectroscopic Methods) and CHM 408 (Organic Reactions and Synthesis), Obafemi Awolowo University, Ile-Ife, Nigeria

Student Chemical Society of Nigeria Prize for the best graduating student in Chemistry, Obafemi Awolowo University, Ile-Ife, Nigeria

Community Service

Young African Voices for Peace Initiative, September 2010 – present, Publicity Secretary, Board of Trustees. A non-profit organization that has been involved in mobilizing and uniting young Africans at home and in diaspora toward peace promotion, youth engagement and empowerment, and community service.

Volunteered with Life Tutors in Nigeria to teach chemistry, mathematics, and physics for freshmen and sophomore students from 2002 to 2007. I also conducted and coordinated exams.

I was the assistant publicity manager for a campus-wide campaign tagged "Say No and Act Right" at the Obafemi Awolowo University in Nigeria. It was a national initiative intended to increase awareness of the campus community in areas of academic honesty, ethical standards, and the need for respectful treatment of one another.