

AMARACHI G. SYLVANUS

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SUMMARY

A highly motivated doctoral candidate in computational chemistry with over 3 years of experience in electronic structure theory calculations and quantum chemistry. Strong hands-on experience in problem-solving using techniques like density functional theory (DFT), coupled cluster (CC) theory, molecular dynamics (MD) simulations, and machine learning. Essential proficiency in presenting research updates and summaries through reports, presentations, and publications in scientific journals. Quick learner, attention to detail, and ability to provide mentorship to undergraduate research students.

EDUCATION

The University of Tennessee– Knoxville, TN

Doctor of Philosophy in Chemistry

University of Ibadan – Ibadan, Nigeria

Bachelor of Science in Chemistry

Graduation: 12/25

GPA: 4.0/4.0

Graduation: 05/19

GPA: 3.6/4.0

(First-class Honors)

SKILLS

Computational Tools: TURBOMOLE, Gaussian, ORCA, LAMMPS, Pyscf, Mathematica

Programming Languages: Python

Theory Methods: Density Functional Theory, Coupled-Cluster Theory, Molecular Dynamics simulation.

Interpersonal Skills: Problem-solving, Teamwork, Leadership, Time management, Decision making.

Analytical Skills: Machine learning, Data analysis, Data visualization.

RELATED EXPERIENCE

Graduate Teaching and Research Assistant, Department of Chemistry

01/2021 – Present

The University of Tennessee– Knoxville, TN

Advisor: Dr. Konstantinos Vogiatzis

Computational Examination of Biomimetic Capture of CO₂ with Oligopeptides

- Performed accurate quantum study of the interaction of amino acid and CO₂ towards sustainable atmospheric gas capture.
- Performed benchmarking studies of different density functionals against coupled cluster results.
- Developed a machine learning model for the prediction of electronic structure properties of larger oligopeptides using chemically driven persistent homology.
- Taught undergraduate chemistry labs, provided tutorial office hours to students, and graded weekly quizzes and monthly examinations.
- Student mentor for the UT-ORII-2023 Student Mentoring and Research Training (SMaRT) program

Undergraduate research, Department of Chemistry

03/2019-05/2019

University of Ibadan– Oyo, Nigeria

Advisor: Prof. B.B. Adeleke

Experimental and Computational Analysis of Schiff Bases from Pyridine Derivatives

- Synthesis of pyridine and pyrazine derivatives Schiff bases.
- Theoretical and spectroscopic analyses of these Schiff bases for pharmaceutical uses.
- Prediction of molecular descriptors, and geometric parameters that characterize these compounds for drug discovery.

SAAG Chemical Nigeria Limited

02/2018-04/2018

Lagos, Nigeria

- Physiochemical analysis of foods, chemicals, and consumer use produce for quality control purposes.
- Analysis of wastewater from industries for environmental inspection.

PRESENTATIONS/CONFERENCES

- **Amarachi G. Sylvanus** and Konstantinos Vogiatzis. "Accurate Interaction Energies of CO₂ with the 20 Naturally Occurring Amino Acids" *SETCA, Atlanta*, May 19-21, 2022.
- **Amarachi G. Sylvanus** and Konstantinos Vogiatzis. "Computational Examination of Interaction of CO₂ with Oligopeptides for Biomimetic CO₂ Capture" *SETCA, Columbia*, May 11-13, 2023.
- **Amarachi G. Sylvanus** and Konstantinos Vogiatzis. "Computational Examination of Interaction of CO₂ with Oligopeptides for Biomimetic CO₂ Capture" *Chemical Separations GRC, Galveston TX*, January 21-26, 2024.
- **Amarachi G. Sylvanus**, Grier Jones, Radu Custelcean and Konstantinos Vogiatzis. "Computational Examination of Interaction of CO₂ with Oligopeptides for Biomimetic CO₂ Capture" *SETCA, Blacksburg*, May 16-18, 2024.

PUBLICATIONS

- **Sylvanus, A. G.**, & Vogiatzis, K. (2023). Accurate Interaction Energies of CO₂ with the 20 Naturally Occurring Amino Acids. *ChemPhysChem*, e202300027.
- **Sylvanus, A.**, Jones, G., Custelcean, R., Vogiatzis, K. (2024). In Silico Screening of CO₂-Dipeptide Interactions for Biomimetic Carbon Capture. *Environ. Sci. Technol.* In review.

MEMBERSHIPS

- American Chemical Society (ACS) Membership number: 32983160
- National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCCChE)

SELECTED AWARDS AND RECOGNITION

- Outstanding Ph.D. candidate award, Department of Chemistry, UTK 05/2023
- Dean's Roll of Honors Award for first-class students, Faculty of Science, University of Ibadan 10/2018
- Member of the year, Association of Chemistry Graduate Students (ACGS, UTK) 05/2024

VOLUNTEERING EXPERIENCE

HIV/AIDS Community Development Service, National Youth Service Corps 07/2019-02/2020
Ilorin, Nigeria

- Community outreach and sensitization in local markets and public schools on the myths and facts of HIV/AIDS and similar STDs.
- Free HIV testing and follow-up counseling.
- Provision of free 'barrier' method of contraception for indigenes of the community.

Tennessee State Science Olympiad

Event Supervisor: Core knowledge (meteorology) 04/01/2023

- Volunteered as an Event Supervisor, offering guidance to contestants, managing event examinations, and resolving tiebreakers in core knowledge assessments.

Nigerian Student Association (NSA), The University of Tennessee chapter 06/2023 – Present
Welfare committee chairperson

- Orientation of incoming Nigerian students on housing and transportation concerns
- Provided a database of apartments and houses that meet the price and proximity range for incoming Nigerian students.
- Assisted in communicating the needs and welfare of new students to the general student body.

Association of Chemistry Graduate Students (ACGS), UTK 08/2023 – Present
Philanthropy and Service Chair

- Led a team effort to volunteer with 'Our Place Art' for their annual fundraising event, dedicated to supporting individuals with autism.

International Student Affairs Chair

- I conducted an orientation meeting for first-year international students, addressing inquiries and providing guidance on navigating graduate school successfully as an international student.