GEORGE BAFFOUR PIPIM

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PROFESSIONAL SUMMARY

Computational chemist specializing in quantum chemistry, excited-state dynamics, and spectroscopic simulations. Applied DFT/TD-DFT, CC/EOM-CC, AIMD, and X2C methods to catalysis, photophysics, and electrospray propulsion challenges. Designed and validated models that reproduce experimental spectra (e.g., XAS/XCD, UV–Vis) and guided molecular design for CO_2 photoreduction, OLED emitters, and metalloporphyrins. 18 peer-reviewed publications, multiple fellowships/awards; experienced collaborator with experimental teams; proficient across Q-CHEM, Schrödinger Software Suite, ORCA, Gaussian, and Python workflows.

EDUCATION

University of Southern California, USC, Aug 2021 – May 2026

Doctor of Philosophy in Chemistry
Advisor: Prof. Anna I. Krylov

University of Southern California, USC, Aug 2021 – May 2024

Master of Arts in Chemistry
Advisor: Prof. Anna I. Krylov

Kwame Nkrumah University of Science and Technology, KNUST, Sep 2016 – June 2020

Bachelor of Science in Chemistry, **First Class Honors**, Class Rank: **1/247**
Thesis title: "Quantum Mechanical Studies on the Mechanisms of Selected 1,3-Dipolar Cycloaddition Reactions for the Formation of Synthetically- and Pharmaceutically Relevant Precursors"
Advisors: Prof. Richard Tia and Prof. Evans Adei

SKILLS

- Methods: Couple cluster methods, Density functional methods, Ab initio Molecular dynamics, Non-adibatic dynamics
- Programming/Libraries: Python, PyTorch, Numpy, Pandas, Matplotlib, Scipy, Sci-kit Learn, Rdkit, Linux Bash, Jupyter, Slurm
- Software: Q-CHEM, Schrödinger Software Suite, Gaussian, ORCA, GaussView, Spartan, JMOL, Iqmol, Discovery Studio

RESEARCH EXPERIENCE

Krylov's Group, University of Southern California Los Angeles, CA
Graduate Research Assistant Aug 2021 – present

- Developed and validated AIMD workflows to study field- and collision-induced fragmentation in EMI–BF_4 propellants; quantified picosecond soft-fragmentation pathways and identified energy thresholds for bond cleavage, informing multiscale thruster models.
- Benchmarked excited-state methods (TD-DFT vs. EOM-CC) to model photophysics of oligo-*p*-phenylenes (OPPs) used in CO_2 photoreduction; identified ωPBE as the most reliable functional for reproducing optical and excitonic properties, enabling predictive screening of functionalized terphenyls with enhanced radical anion generation and extended fluorescence lifetimes.
- Applied relativistic quantum chemistry (X2C) to investigate Au, Cu, and Ag OLED complexes; reproduced experimental optical and electronic properties and established a predictive framework for the rational design of next-generation emitters for display applications.
- Mapped relaxation pathways of cobalt metalloporphyrins using ab initio molecular dynamics (AIMD) with fewest-switch surface hopping; identified energetically favorable fragmentation channels consistent with ultrafast photodissociation experiments, clarifying competing excited-state relaxation mechanisms.
- Simulated core-level X-ray absorption and circular dichroism (XAS/XCD) spectra of hydrocarbons using EOM-CCSD; assigned spectral features to underlying electronic transitions, providing theoretical insight to support experimental interpretation.
- Built Python tooling to automate job submission, result parsing, and analysis across Q-CHEM/CFOUR/ORCA on Slurm-managed clusters, reducing setup time and human error

Molecular Modeling Group, Kwame Nkrumah University of Science and Technology Kumasi, Ghana
Research Assistant Jan 2019 – Aug 2021

- Investigated the mechanisms of key organic reactions involved in the design and synthesis of pharmaceutical intermediates and fine chemicals using density functional theory (DFT). Constructed detailed potential energy surfaces to identify transition states, intermediates, and substituent effects governing regio-, stereo-, and chemoselectivity. Derived mechanistic insights that rationalize experimental outcomes and inform the development of more efficient and selective synthetic routes..

- Designed and optimized Pt- and Pd-based catalysts for biomass conversion using density functional theory (DFT); investigated reaction mechanisms, active-site energetics, and ligand effects to elucidate structure–activity relationships and guide the development of more efficient catalytic systems for sustainable transformations.
- Performed molecular docking and interaction analysis of small-molecule inhibitors within the active sites of disease-related proteins; characterized key binding interactions and conformational changes to support structure-based drug design and lead optimization.

TEACHING EXPERIENCE

Teaching Assistant (20 hours per week), Department of Chemistry, USC Aug 2021 - present
- Supervised Organic (322A) and Advanced General Chem. (115A, 115B) lab sessions
- Graded tests and assignments of undergraduate students for Organic (322A) and Advanced General Chem. (115A, 115B)
- Organized office hours for undergraduate students to discuss lab concepts.

Teaching Assistant (20 hours per week), Department of Chemistry, KNUST Aug 2020 – Aug 2021
- Graded tests and assignments of undergraduate students for Physical Chemistry (155, 156 355, 356 & 473)
- Organized supplementary instruction (Physical Chemistry) for undergraduate students to discuss class concepts
- Instructed Analytical and Inorganic Chemistry (169, 170, 269 & 270) undergraduate lab courses

Science and Mathematics Teacher (40 hours per week), Jesus Grace Academy May 2015 - Aug 2018
- Instructed junior high school students in general science and mathematics
- Organized and supervised science practical sessions to strengthen students' experimental and analytical skills.
- Prepared instructional materials and assessments to support effective learning outcomes.
- Assisted in school information technology operations and digital classroom resources.

MEMBERSHIP IN PROFESSIONAL ASSOCIATIONS

- American Chemical Society (ACS) - Member
- Ghana Chemical Society (GCS) - Member
- National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE) - Member
- International Younger Chemist Network (IYCN) - Member

HONORS AND AWARDS

- Advancing Science Conference Grant, Tier One, (2025)
- Advancing Science Conference Grant, Tier One, (2024)
- Dornsife/Graduate School Fellowship Award (2023), USC
- Chemistry Diversity Graduate Fellowship Award (2021), Department of Chemistry, USC
- Overall Best Graduating Chemistry Student Award (2020), Department of Chemistry, KNUST
- Outstanding Undergraduate Researcher Award (2020), Department of Chemistry, KNUST
- Best Male Graduating Chemistry Student Award (2020), Department of Chemistry, KNUST

MENTORING AND SERVICE WORK

- Peer Reviewer, Scientific Journals & Conferences: Provided peer reviews of journal manuscripts and evaluated abstracts submitted to chemistry-related conferences
- Research Student Mentor (KNUST & USC): Mentored incoming research students by training them in lab protocols, computational tools, and active projects, and providing ongoing academic and scientific guidance
- Q-Chem User Workshop (Winter Virtual School) — mentored participants during live computational exercises and provided real-time technical support for Q-Chem simulations.
- USC Chemistry Recruitment Guide: Assisted with hosting and guiding prospective students and supported departmental outreach activities
- Program Officer, TopGates Africa: Assisted in planning and coordinating programs aimed at improving education in rural communities
- Peer Counsellor, Science Students' Association, KNUST: Provided academic and personal guidance to first-year students
- Chairman, Academic Committee, Ghana Students' Chemical Society, KNUST (2019–2020): Organized academic support and mentorship programs for first-year chemistry students

SELECTED CONFERENCES AND WORKSHOPS

- ***Conference***: "NOBCChE's 52nd Annual Meeting, Hilton Hotel in Atlanta, Georgia, (September 2025), oral presentation
- ***Conference***: " DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting in Rockville, Maryland, (August 2025), poster presentation
- ***Conference***: "NOBCChE's 51st Annual Meeting, Rosen Shingle Creek in Orlando, Florida, (September 2024), oral presentation
- ***Conference***: "The 50th John Stauffer Conference", by Department of Chemistry, University of Southern California (April 2024), poster presentation
- ***Workshop and Conference***: "Modern Wavefunction Methods Summer School" by Department of Chemistry, University of Pisa, Italy (August 2023), poster presentation
- ***Conference***: "West Coast Theoretical Chemistry Meeting", by Department of Chemistry, University of California, Davis (May 2023), poster presentation
- ***Conference***: "The 49th John Stauffer Conference", by Department of Chemistry, University of Southern California (March 2023), poster presentation
- ***Conference***: "International Virtual Conference on Chemistry and its Application: Schrödinger Day and International Youth Day, Elsevier Research Building Capacity", by the Department of Chemistry, University of Mauritius (August 2020).
- ***Conference***: "International Conference on Materials for Renewable and Sustainable Energy: From Research to Development, Research Workshop for Students", by the Royal Society of Chemistry - Africa Capacity Building Initiative, Amonoo-Neizer Conference Center, Kumasi, Ghana (June 2019), poster presentation

PUBLICATIONS

1. Sampson D. K., **Baffour Pipim, G.**, Noah Tingey N., Torres J., Depew D., Wang J and Krylov I. A., *Collision-Induced Fragmentation of the EMI-BF4 Propellant in Electrospray Thrusters: ab initio Molecular Dynamics Simulations* (*Under review at Journal of Chemical Physics*)
2. **Baffour Pipim, G.**, Sampson D. K., Noah Tingey N., Torres J., Depew D., Wang J and Krylov I. A., *Ab initio simulations of dynamics of EMI-BF4 ionic liquid propellant used in electrospray thrusters for nanosatellite applications* (*J. Chem. Phys. 163, no. 22 (2025).*)doi.org/10.1063/5.0296441
3. **Baffour Pipim, G.**, Sharada, S.M., Krylov, I. A. (2025). *Photophysical properties of functionalized terphenyls and implications to photoredox catalysis.* Pure Appl. Chem., 2025. doi.org/10.1515/pac-2025-0560
4. Sampson D. K, **Baffour Pipim, G.**, Noah Tingey N, Torres J, Depew D., Wang J. and Krylov I. A, *Exploring collision-induced fragmentation in porous electrospray thrusters*, 38th IEPC-2024-613, Conference paper, doi:383983879_Exploring
5. Patra A, **Baffour Pipim G.**, Krylov I. A., Sharada S.M. *Performance of density functionals for excited-state properties of isolated chromophores and exciplexes: Emission spectra, Solvatochromic shifts, and charge-transfer character*. J.Chem. Theo. Comp. 2024, doi.org/10.1021/acs.jctc.4c00005
6. Atta-Kumi, J., **Baffour Pipim, G.**, Opoku, E., *Tandem [4+2]/retro[3+2]/[3+2] cycloaddition reactions of fluorinated-oxadiazoles with conjugated, unconjugated, cyclic, and acyclic dienes*, J Phys Org Chem 2023, doi.org/10.1002/poc.4567
7. **Baffour Pipim, G.**, Opoku E., *Catalyst-free (3 + 2) cycloaddition reaction of oxa-, aza-, and thio-bicyclic alkenes with cyclic and acyclic nitrones: A mechanistic study* Comput. Theor. Chem., 2022, 1124, 113790 p. doi.org/10.1016/j.comptc.2022.113790
8. Fosu, A., **Baffour Pipim, G**., Tia, R. and Adei, E., *Does the reaction of nitrone derivatives with allenoates proceed by an initial (3 + 2) cycloaddition or O-Nucleophilic addition? A quantum chemical investigation*, J. Mol. Graph. Model., 2021, 109, 108036 p. doi.org/10.1016/j.jmgm.2021.108036
9. Tawiah A., **Baffour Pipim, G**., Tia, R. and Adei, E., *Exploring the chemo-, regio-, and stereoselectivities of the (*$3+2$*) cycloaddition reaction of 5,5-dimethyl-3-methylene-2-pyrrolidinone with C,N-diarylnitrones and nitrile oxide derivatives: a DFT study*, J Mol Model 27, 287, 2021. doi.org/10.1007/s00894-021-04911-0
10. Ofori, I., **Baffour Pipim, G.**, Tia, R. and Adei, E., *A DFT study of the double (3 + 2) cycloaddition of nitrile oxides and allenoates for the formation of spirobiisoxazolines*, J. Mol. Graph. Model., 2021, 109, 108033 p, doi.org/10.1016/j.jmgm.2021.108033
11. Atta-Kumi, J., **Baffour Pipim, G.**, Tia, R. et al. *Investigating the site-, regio-, and stereo-selectivities of the reactions between organic azide and 7-heteronorbornadiene: a DFT mechanistic study*. J Mol Model 27, 248 (2021). doi.org/10.1007/s00894-021-04857-3
12. **Baffour Pipim, G.**, Tia, R. and Adei, E., *Quantum Chemical Investigation of the Formation of Spiroheterocyclic Compounds Via the (3 + 2) Cycloaddition Reaction of 1-methyl-3-(2,2,2- trifluoroethylidene)pyrrolidin-2-one with Diazomethane and Nitrone Derivatives*, Tetrahedron, 2021 doi.org/10.1016/j.tet.2021.132306.

13. **Baffour Pipim, G.**, Opoku, E. *Unveiling the molecular mechanisms of the cycloaddition reactions of aryl hetaryl thioketones and C,N-disubstituted nitrilimines*. J Mol Model 27, 84, 2021. doi.org/10.1007/s00894-021-04706-3
14. **Baffour Pipim, G.**, Tia, R. and Adei, E., *Computational Exploration of the 1,3-Dipolar Cycloaddition Reaction of 7-Isopropylidenebenzonorbornadiene with Nitrile Oxide and Cyclic Nitrone Derivatives*, J. Phys. Org. Chem., Wiley, 2020 e4174, doi.org/10.1002/poc.4174
15. **Baffour Pipim, G.**, Tia, R. and Adei, E., *(3 + 2) Cycloaddition Reaction of 7- Isopropylidenebenzonorbornadiene and Diazomethane Derivatives: A Theoretical Study*, J. Mol. Graph. Model, 2020, 101, p. 107713. doi.org/10.1016/j.jmgm.2020.107713.
16. **Baffour Pipim, G.**, Tia, R., and Adei, E., *Investigating the Regio-, Stereo-, and Enantio-Selectivities of the 1,3-Dipolar Cycloaddition Reaction of C-cyclopropyl-N-phenylnitrone Derivatives and Benzylidenecyclopropane Derivatives: A DFT Study*, J. Mol. Graph. Model., 2020, 100, p. 107672.doi.org/10.1016/j.jmgm.2020.107672
17. **Baffour Pipim, G**., Opoku, E., Tia, R. and Adei, E., *Peri-, Chemo-, Regio-, Stereo- and Enantioselectivities of 1,3-Dipolar Cycloaddition Reaction of C,N-disubstituted Nitrones with Disubstituted 4-methylene1,3-oxazol-5(4H)- one: A Quantum Mechanical Study*, J. Mol. Graph. Model., 2020, 97, p.107542. doi.org/10.1016/j.jmgm.2020.107542.
18. Opoku, E., **Baffour Pipim, G.**, Tia, R. and Adei, E., *Mechanistic study of the Tandem intramolecular (4 + 2)/intermolecular (3 + 2) cycloaddition reactions for the Formation of Polyaza-and polyisoxazolidine- steroids*. J. Heterocycl. Chem, 2020. 57(4), pp.1748-1758. doi.org/10.1002/jhet.3900.
19. Opoku, E., Arhin, G., **Baffour Pipim, G.**, Adams, A.H., Tia, R. and Adei, E., *Site-, Enantio- and Stereoselectivities of the 1,3-Dipolar Cycloaddition Reactions of Oxanorbornadiene with C,N disubstituted Nitrones and Dimethyl Nitrilimines: A DFT Mechanistic Study*, Theor. Chem. Acc. 2020 139(1), pp.1-15. doi.org/10.1007/s00214-019-2529-8