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JOSEPH FRIMPONG

Wayne State University

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Summary

A motivated Ph.D. candidate with 5+ years of experience in computational chemistry, programming, and machine learning. Proficient in Python and data analytics, I also have a strong background in method development and molecular dynamics simulations. I work well independently and in teams, and am eager to apply my skills to applied research. My background in chemistry and physics makes me a valuable asset for addressing germane research challenges.

Education

PhD in Chemistry, *Wayne State University* 2019-2023
Major: Physical Chemistry Detroit, MI
Masters of Arts, *Wayne State University* 2019-2021
Major: Chemistry Detroit, MI
Bachelor of Science in Chemistry, *Kwame Nkrumah University of Science and Technology* 2013-2017
Major: Computational Chemistry Kumasi, GH

Skills

Programming Languages	Python, C++, FORTRAN, OCTAVE, Bash Scripting, Arduino
Modelling Software	Quantum ESPRESSO, AMBER, TeraChem, Gaussian, BerkeleyGW, GROMACS, LAMMPS, PySCF
High-Performance Computing	Supercomputers[NERSC, XSEDE (TACC, PSC bridges, & Expanse), BNL, ANL (Carbon), WSU Grid]
Visualization Software	VESTA, XCrySDen, Avogadro, VMD, ASE, GNUplot, GaussView, BURAI, Matplotlib, Origin, MATLAB
Technical Skills	NumPy, Pandas, Machine Learning & Data Science [KERAS, Scikit-learn, TensorFlow, Tableau]
Instrumentation	UV-VIS, GC-MS, LC-MS, TLC, HPLC, IR, Microcontrollers & Embedded Device Engineering (ESP32, ESP8266, Arduino, Raspberry Pi)
Operating Systems	Linux, Windows, Mac
Communication	English, Twi (fluent speaker), French (written)

Research Experience (Selected Projects)

PROJECT 1: Quasiparticle electronic structure and optical properties of modern Quantum materials **Sept 2020 - Present**
Wayne State University | PI: Zhenfei Liu funded by *Detroit, MI*

- Pioneered a novel GW/BSE method for studying large heterogeneous interfaces with **programming tools** like **(FORTRAN, Python, BASH)** while **implementing machine learning techniques** to enhance research efficiency
- Employed ab-initio computational methods, including DFT and GW/BSE, to probe various industrially pertinent materials, including Covalent Organic Frameworks, Quantum Dots, and Organic-Metal Interfaces, contributing to an enhanced understanding of semiconductor-related properties.
- Proficiently **troubleshooted computing systems**, including supercomputers, ensuring uninterrupted research operations and the maintenance of high-performance computing environments.
- Created custom scripts tailored to streamline research workflows, resulting in improved data analysis and visualization capabilities.
- Applied advanced **data analysis** and **graphical visualization** techniques to extract valuable insights into complex structure-property relationships, facilitating informed decision-making in materials design and optimization

PROJECT 2: Interfacial studies of CO_2 reduction on graphene-Fe interfaces **2018 - 2021**
Kwame Nkrumah University of Science and Technology | PI: Dr. Caroline Kwawu *Kumasi, GH*

- Elucidated the reduction mechanism of CO_2 to CO on graphene-Fe (100) interface using DFT [Quantum ESPRESSO]

PROJECT 3: Mechanistic studies of the reaction alkynyl phosphates with norbornadiene **2016 - 2017**
Kwame Nkrumah University of Science and Technology | PI: Prof. Evans Adei & Dr. Richard Tia *Kumasi, GH*

- Investigated the Ru-catalyzed mechanism to optimize the reaction yield and selectivity using computational methods [Gaussian 09 and Spartan 14 codes]

Publications

- Aryal* S., **Frimpong* J.**, and Liu Z.(2023) *Understanding the ligand exchange in CdS quantum dots from first principles* (Under Preparation)
- **Frimpong J.** and Liu Z. (2023) *Extending the substrate screening GW approximation to covalently bound interfaces* (Submitted)
- Behera N., Gunasekera D., Mahajan J., **Frimpong J.**, Liu Z, Luo L. (2023) *Electrochemical Hydrogen Isotope Exchange of Amines Controlled by Alternating Current Frequency*, Faraday Discuss. Accepted Manuscript [link]

- Aryal S.*, **Frimpong J.*** and Liu Z.(2022) *Comparative Study of Covalent and van der Waals CdS Quantum Dot Assemblies from Many-Body Perturbation Theory*, J. Phys. Chem. Lett. 2022, 13, 43, 10153–10161 [link]
- **Frimpong J.** and Liu Z. (2021) *"Quasiparticle electronic structure of two-dimensional heterotriangulene-based covalent organic frameworks adsorbed on Au(111)"* J. Phys.: Condens. Matter **33**, 254004 [link]

Awards and Honors

- NOBCChE Advancing Science Conference Award (2022-2023)
- Summer Dissertation Award - Wayne State University (2023)
- Energy Research Travel Funding (GERA), APS March Meeting, Chicago, IL (2022,2023)
- A. Paul and Carole C. Schaap Endowed Distinguished Graduate Award (given to top graduate students in Chemistry) (2022)
- Thomas C. Rumble Fellowship Award (in recognition of superior academic achievement in research) (2022)
- Best Poster Award - Computational Chemistry, NOBCChE National Conference (2022)
- ICTP Travel Award - The Abdus Salam International Centre for Theoretical Physics, Italy (2019)
- KBN Merit Scholarship Kwame Nkrumah University of Science and Technology, Italy (2019)

Teaching Experience

Graduate Teaching Assistant, *Wayne State University* Sept 2019 – Present

- Led a discussion class for freshmen in foundational general chemistry courses (CHEM 1220)

Physics/Chemistry Teacher, *Tamale Senior High School* Nov 2018 – Aug 2019

- Taught, assessed, and graded 210 high school students in general chemistry and physics. **Improved the percentage pass rate from 50 to 86% in annual exam**
- Demonstrated, supervised, and developed student-centered laboratory sessions in chemistry and physics

Teaching Assistant, *Kwame Nkrumah University of Science and Technology* Sept 2018 – Aug 2018

- Taught experimental inorganic chemistry courses
- Taught students the technical know how of UV, MS, IR and HPLC instruments to perform molecular structural elucidation

Conferences and Presentations (selected)

- **J. Frimpong** and Z. Liu (2023) Development of GW-based substrate screening methods for covalently-bound interfaces, NOBCChE National Conference 2023, September 12, New Orleans, LA
- **J. Frimpong**, and Z Liu (2023) Development of GW-based substrate screening methods for strongly coupled molecule-metal interfaces, APS March Meeting 2023, March 18, Las Vegas, NV
- **J. Frimpong**, S. Aryal, and Z. Liu (2022) Unraveling the role of Surface Ligands in the Electronic and Optical Properties of Cadmium Sulphide Quantum Dots, NOBCChE National Conference 2022, September 25, Orlando, FL
- **J. Frimpong**, S. Aryal, and Z. Liu (2022) Electronic Structure and Optical Properties of Quantum Dots their Assemblies, APS March Meeting 2022, March 18, Chicago, IL
- **J. Frimpong** and Z. Liu (2021) Electronic structure of 2D-covalent organic frameworks and the influence of Au(111) substrate, Chemistry Graduate Research Symposium (CGRS), Detroit, MI. (Student Talk)
- **J. Frimpong** and Z. Liu (2021) Quasiparticle electronic structure of two-dimensional heterotriangulene-based covalent organic frameworks adsorbed on Au(111), APS March Meeting 2021, March 17 (Virtual)
- **J. Frimpong** (2019) Mechanistic studies of the cycloaddition of norbornadiene and alkynyl phosphonates, 19th International Workshop on Computational Physics and Material Science, Trieste, Italy (Poster Presentation)

Certifications

Courses on data science, machine learning, and deep learning in Coursera, Datacamp, and at Wayne State University.

Online courses completed: Machine Learning; Neural Networks & Deep Learning; Improving Deep Neural Networks; Data Science in Python

Wayne State: WSU Data Science Certification, **DSA 6000** (Data Science & Analytics), **IE 6010** (IoT and Edge AI Programming)

MENTORSHIP

Tejas Karun, BS Chemistry *WSU '23* Winter 2022-Present

- Designed and supervised project: Electronic Structure studies of 2DPA-1 using Density Functional Theory Studies (DFT)

Lyric Elliott , BS Chemistry *WSU '21* Winter 2022-Present

- Designed and supervised project: Electronic Structure studies of quinoidal polymers using DFT

Leadership Experience

- **Social Media Coordinator** (Aug 2022 - July 2023) WSU NOBCChE Chapter
- **NOBCChE's K-12 Initiative**(2021-2023) Detroit Public School, Detroit, MI, USA
- **NOBCChE Conference Planning Committee**(2022 – Present)
- **Facilitator** - Chemistry Meets Computers - Coding Summer Camp (2021, 2022, 2023) Wayne State University, Detroit, MI, USA
- **General Secretary** (Aug 2021 - July 2022) WSU NOBCChE Chapter
- **Volunteer** (Oct 2021, Nov 2023) Detroit Public School Outreach
- **Volunteer** (March 2023) Neinas Chemistry Outreach
- **Peer Reviewer** for Journal of Physics: Condensed Matter, Physical Review B, Physical Review Letters, IOP Physica Scripta

Professional Membership

American Physical Society **(APS)** (2019-Present) | American Chemical Society **(ACS)**(2019-Present) | National Organization for the Professional Advancement of Black Chemists and Chemical Engineers **(NOBCChE)** (2019-Present) | Ghana Student Chemical Society **(GSCS)** (2013-2019) | Royal Society of Chemistry **(RSC)** (2014-2019)

References

- **Dr. Zhenfei Liu** [Advisor]
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