RAPHAEL NNAEMELUM OGBODO

Iowa City, IA 52246 | Phone: +1 (319) 855-9987 | Email: raphaelogbodo4@gmail.com
Google Scholar | LinkedIn | GitHub | Huggingface

EDUCATION

PhD in Chemistry (Physical and Computational)
University of Iowa, Iowa City, IA | (**Expected 2026)**

- ✓ **Dissertation Title**: Structure, dynamics, and transport properties of room temperature ionic liquids, zwitterions, and molten salts in extreme environments
- ✓ **Advisor**: Prof. Claudio J. Margulis

M.Sc. in Chemistry (Physical and Computational)
University of Iowa, Iowa City, IA | 2023

- ✓ **Advisor**: Prof. Claudio J. Margulis

B.Sc. in Pure and Industrial Chemistry (First Class Honors, GPA (4.58/5.0))
University of Nigeria, Nsukka | 2017

- ✓ **Thesis**: Production of bioethanol from plantain and banana peels and their comparative mineral element analysis
- ✓ **Advisor**: Prof. Samson Ifeanyi Eze

PROFESSIONAL EXPERIENCE

Gained as a Graduate Research and Teaching Assistant, University of Iowa | 2021–Present

- **Computational Modeling & Simulations:**
  - ✓ **Method Development & Multiscale Modeling:**
    Developed **novel computational methodologies** to extract structural, dynamical, and transport properties from **classical molecular dynamics (GROMACS)** and **first-principles quantum simulations (CP2K)**, enabling quantitative interpretation of experimental scattering data and demonstrating transferable approaches applicable to molecular, biological, and materials systems.
  - ✓ **Advanced Molecular Simulation & Force Field Application:**
    Performed **polarizable force-field molecular dynamics simulations** and **analyzed trajectories generated using machine-learned DFT-based interatomic potentials** developed in collaboration with national laboratory partners, modeling complex condensed-phase systems under challenging conditions and demonstrating expertise in high-fidelity molecular simulation workflows relevant to drug discovery, soft matter, and chemically complex environments.
  - ✓ **Integrated Physics-Based Modeling & Machine Learning:**
    Completed **Schrödinger's Applied Molecular Modeling certification**, developing hands-on expertise in **classical MD, molecular and periodic quantum mechanics, and ML-driven property prediction workflows** (Desmond, Jaguar, AutoQSAR, Maestro) for **multiscale computational studies across chemical, biological, and materials systems**.
  - ✓ **Cross-Disciplinary Collaboration, Leadership & Scientific Communication:**
    Led and contributed to **multidisciplinary collaborations** with experimental scientists and national laboratory partners, translating computational results into actionable physical insight. Co-authored **5 peer-reviewed publications** and contributed to **1 NSF-funded project**, demonstrating strong mentorship, leadership, and written communication skills.

- **Data Science & Machine Learning:**
  - ✓ **Advanced Deep Learning & Representation Learning:**
    Completed a graduate-level Deep Learning course (A+ grade) covering modern neural architectures including **CNNs, RNNs, Transformers, Autoencoders/VAEs, GANs, and Reinforcement Learning**. Designed and implemented a **CNN-based representation learning model with a novel triplet-loss variant** for supervised image classification, achieving **0.98 accuracy and strong F1 performance** on a medical imaging task, demonstrating robust feature learning and generalization on real-world data.

  - ✓ **Graph Neural Networks & Transfer Learning:**
    Designed and implemented **message-passing GNNs in PyTorch** for predictive modeling on structured data, achieving low error across multiple continuous targets. Applied **transfer learning** to related domains, demonstrating the model's ability to learn reusable, domain-agnostic representations. Built graph-based features using **RDKit and OpenBabel**, highlighting strengths in representation learning for complex relational data.

  - ✓ **End-to-End Machine Learning & Data Science Pipelines:**
    Earned the **IBM Data Science Professional Certificate (Coursera)**, completing an end-to-end ML capstone involving data wrangling, feature engineering, model training, validation, and deployment-oriented analysis. Implemented and compared multiple supervised learning algorithms (**Logistic Regression, SVM, KNN, Random Forest**), achieving **0.98 accuracy**, and strengthening proficiency in **Python (scikit-learn, pandas, numpy), SQL, data visualization, and cloud-based analytics workflows**.

  - ✓ **AI for Scientific & High-Performance Computing Applications:**
    Participated in the **NERSC End-to-End AI for Science Bootcamp** (NERSC / NVIDIA / OpenACC), gaining hands-on experience with **data-driven and physics-informed neural networks**, model visualization, and scalable AI workflows for scientific computing environments using **NVIDIA Modulus** and HPC-oriented tooling.

- **Teaching**:
  - ✓ Instructed 600+ undergraduate students annually in general and advanced chemistry topics; mentored students in laboratory techniques and research methods.
  - ✓ Evaluated student assignments, laboratory reports, and examinations with constructive feedback.

Gained as Graduate Assistant Lecturer, University of Nigeria, Nsukka | 2019–2021
- ✓ Instructed 1000+ undergraduate students in chemistry practical courses across five specializations (organic, inorganic, physical, analytical, industrial).
- ✓ Developed and delivered laboratory protocols, practical sessions, and assessments with 90%+ student pass rates.
- ✓ Provided academic support and tutoring to resident students.
- ✓ Contributed to departmental administration and curriculum development.

Gained as Laboratory Assistant, Federal Polytechnic, Ebonyi State, Nigeria | 2018-2019
- ✓ Conducted and supervised ND and HND student chemistry practical sessions.
- ✓ Developed laboratory protocols and assessment materials.

- ✓ Graded practical workbooks and examinations.

Gained as Chemistry Tutor, Doyen Academy and British Cambridge Advanced Level School, Enugu, Nigeria | 2017-2018

- ✓ Taught and prepared advanced-level students for Cambridge A-level examinations.
- ✓ Prepared students for IGCSE and WAEC examinations.
- ✓ Developed course materials and assessment tools.

RESEARCH EXPERTISE AND TECHNICAL SKILLS

Core & Transferable Competencies

Research & Data Analysis | Project & Time Management | Cross-Disciplinary Collaboration | Scientific Communication | Mentorship & Leadership | Rapid Skill Acquisition | Technical Problem Solving

Computational Modeling & Simulation

Classical Molecular Dynamics (GROMACS, LAMMPS, MetalWalls) | Trajectory Analysis (MDAnalysis, VMD, ASE, TRAVIS) | Enhanced Sampling (Replica Exchange MD) | Multiscale & Condensed-Phase Modeling

Quantum Chemistry & Electronic Structure

First-Principles & Periodic QM (CP2K, Gaussian) | DFT-Based Workflows | QM/MM Concepts

Machine Learning & Data Science

Deep Learning & Representation Learning | Graph Neural Networks | Transfer Learning | Supervised & Unsupervised Learning | Model Evaluation & Validation
Python (PyTorch, TensorFlow, Keras, scikit-learn, pandas, NumPy, SciPy, Matplotlib, Seaborn, Plotly) | SQL/MySQL | Dash | Git & GitHub | Generative AI Tools

Cheminformatics & Molecular Representation

RDKit | Open Babel | Molecular Graph Construction | Feature Engineering for ML Models

High-Performance & Scientific Computing

Linux/Unix | HPC Environments | Bash | Fortran | Parallel & Batch Workflows

---

PUBLICATIONS

Book Chapters

1. Okon, E. N.; **Ogbodo, R.**; et al. Ecotoxicological Aspects of Nanotechnology. *Nanotechnology for Sustainable Agriculture, Food, and Environment*; Taylor & Francis Group, 2023.

Peer-Reviewed Journal Articles

1. **Ogbodo, R.**; Margulis, C. J.; et al. Tethered from the Head and from the Tail: The Structure of Hydroxyl-Functionalized Ionic Liquids. *The Journal of Physical Chemistry Letters* 2025, 16,12982–12988. DOI: 10.1021/acs.jpclett.5c03046
2. **Ogbodo, R.**; Margulis, C. J.; et al. Structure of Novel Phosphonium-Based Ionic Liquids with S and O Substitutions from Experiments and a Mixed Quantum-Classical Approach. *The Journal of Physical Chemistry B* **2025**, *129*(14), 3691-3701. DOI: 10.1021/acs.jpcb.5c00129

3. Emerson, M. S.; **Ogbodo, R.**; Margulis, C. J. Spiers Memorial Lecture: From Cold to Hot, The Structure and Structural Dynamics of Dense Ionic Fluids. *Faraday Discussions*, 2024. DOI: 10.1039/D4FD00086B
4. Nnabuk, O. E.; Edet, U. E.; Oladele, J. O.; Kelle, H. I.; Ogoko, E. C.; **Ogbodo, R.**; et al. Synthesis and Application of Novel Microporous Framework of Nanocomposite from Trona for Photocatalysed Degradation of Methyl Orange Dye. *Environmental Monitoring and Assessment*, 2023, *195*(12), 1416. DOI: 10.1007/s10661-023-12014-x
5. **Ogbodo, R.**; Karunaratne, W. V.; et al. Structural Origins of Viscosity in Imidazolium and Pyrrolidinium Ionic Liquids Coupled with the NTf_2^- Anion. *The Journal of Physical Chemistry B*, 2023, *127*(28), 6342-6353. DOI: 10.1021/acs.jpcb.3c02604
6. Eddy, N. O.; Garg, R.; et al. Sol-Gel Synthesis, Computational Chemistry, and Applications of CaO Nanoparticles for the Remediation of Methyl Orange Contaminated Water. *Advances in Nano Research*, 2023, *15*(1). DOI: 10.12989/anr.2023.15.1.000
7. Eddy, N. O.; Ukpe, R. A.; **Ogbodo, R.**; et al. Theoretical and Experimental Studies on Photocatalytic Removal of Methylene Blue (MetB) from Aqueous Solution Using Oyster Shell Synthesized CaO Nanoparticles (CaONP-O). *Environmental Science Pollution Research*, 2023, *30*, 81417-81432. DOI: 10.1007/s11356-022-22747-w
8. Eddy, N. O.; Garg, R.; **Ogbodo, R.**; et al. Application of Periwinkle Shell for the Synthesis of Calcium Oxide Nanoparticles and in the Remediation of Pb^{2+} Contaminated Water. *Research Square Preprint*, 2023. DOI: 10.21203/rs.3.rs-2895593/v1

CONFERENCE PRESENTATIONS

Oral Presentations

1. Musanga cercripodes Wood Sawdust as Intermediate for the Removal of Acid Red Dye from Aqueous Solution. *43rd International Conference of Chemical Society of Nigeria*, Abuja | 2020

Poster Presentations

1. Structure of Trivalent Molten Lanthanide and Actinide Chlorides and Mixtures with NaCl/KCl. *Molten Salts in Extreme Environment All Hands Meeting*, Oak Ridge National Laboratory, Oak Ridge, TN | 2025
2. Calculating the X-ray Structure Function of 1,3 Methylbutylimidazolium Bis-(Trifluoromethylsulfonyl) Amide using Molecular Dynamics Simulations. *Summer School for Integrated Computational Materials Education*, University of Michigan | 2023
3. Structural Dynamics and Viscoelastic Relaxation of Ether and Thioether Substituted Ionic Liquids. *Gordon Research Conference*, Newry, Maine | 2022

Seminar Presentations

1. Understanding the Structure, Dynamics, and Transport properties of Ionic Liquids: A Molecular Dyanamics Simulation Approach. **3-Month Seminar**, *Physical Chemistry Divisional Seminar*, Department of Chemistry, University of Iowa | 2025
2. Computational Analysis of Structure, Dynamics, and Viscoelastic Relaxation of Ionic and Zwitterionic Liquids. *Physical Chemistry Divisional Seminar*, Department of Chemistry, University of Iowa | 2022

FUNDING AND AWARDS

Graduate College Summer Fellowship | University of Iowa | 2025

- ✓ Competitive merit-based award: $5,500

Schrödinger Certification Scholarship | 2025

- ✓ Merit-based award for advanced molecular modeling and ML applications (Value: $575)

PhD Scholarship for Research in Ionic Liquids and Molten Salts | University of Iowa | 2021
- ✓ Competitive award recognizing exceptional academic and research potential

TETFund National Research Fund Award | Nigeria Federal Government | 2020
- ✓ Competitive science/technology/innovation category award
- ✓ Research focus: Development of nano and metal-organic framework adsorbents for water pollution control
- ✓ Project Code: TETF/ES/DR&D-CE/NRF2020/SETI/88/VOL.1

PROFESSIONAL CERTIFICATIONS AND TRAINING

IBM Data Science Professional Certificate | Coursera | 2025
- ✓ **Specialization completion:** Capstone project on machine learning for SpaceX Falcon 9 landing prediction (0.98 accuracy); proficiency demonstrated in Python, Scikit-learn, SQL, and cloud analytics

Schrödinger Applied Battery Materials Certification | Schrödinger | 2025
- ✓ Advanced training in molecular modeling for materials science applications (Desmond, Jaguar, Maestro) and machine learning-based property prediction workflows (AutoQSAR)

NERSC End-to-End AI for Science Bootcamp | NERSC/NVIDIA/OpenACC | 2025
- ✓ Deep neural networks, physics-informed machine learning, and HPC visualization techniques

Summer School for Integrated Computational Materials Education | University of Michigan | 2023
- ✓ Intensive training in computational materials characterization and analysis

---

PROFESSIONAL MEMBERSHIPS

The Scientific Research Honor Society (SIGMA XI) | 2025-Present
American Chemical Society (ACS) | 2024-Present
Chemical Society of Nigeria (CSN) | 2021-Present

LEADERSHIP, MENTORSHIP, AND SERVICE

Graduate Peer-to-Peer Mentor
University of Iowa Graduate Mentorship Program | 2025/2026 Academic Session
- ✓ Direct and guide new graduate students in transition to academic environment
- ✓ Provide information on campus resources and support systems
- ✓ Facilitate problem-solving and adaptation strategies
- ✓ Foster sense of community among new graduate cohort

Road to Recovery Volunteer Driver
American Cancer Society, Iowa City | 2025
- ✓ Provide transportation for cancer patients to medical appointments

STEM Outreach - Chemistry Experiment Booth
Iowa State Fair, Des Moines | 2025
- ✓ Engage public audiences in hands-on chemistry demonstrations
- ✓ Promote interest in STEM and computational science

Presiding Officer
Nigerian General Elections, Ebonyi State | 2019

Public Relations Officer
Environmental Community Development Service, Afikpo North | 2019