Raphael Nnaemelum Ogbodo

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SUMMARY

Computational scientist with 4+ years of experience integrating molecular simulation, quantum chemistry, and machine learning to study complex chemical and biological systems. Proven track record of developing transferable computational methods, analyzing large-scale simulation and experimental data, and collaborating across disciplines, resulting in 9 peer-reviewed publications and NSF-funded research. Strong communicator with experience translating advanced computational insights to experimental and multidisciplinary audiences, with international presentations and leadership in collaborative research projects.

PROFESSIONAL EXPERIENCE

Graduate Research Assistant, The University of Iowa | August 2021 – Present

- **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 Experience

- **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.

EDUCATION

Ph.D. in Computational Chemistry *(Expected 2026)*
The University of Iowa, Iowa City, IA, USA
Focus: molecular simulation, quantum chemistry, scientific machine learning

M.S. in Computational Chemistry *(2023)*
The University of Iowa, Iowa City, IA, USA

B.S. in Pure & Industrial Chemistry *(First-Class Honors) (2017)*
University of Nigeria, Nsukka, Nigeria

SKILLS

Core & Transferable Competencies
Research & Data Analysis | Project & Time Management | Cross-Disciplinary Collaboration | Scientific Communication | Mentorship & Leadership | Rapid Skill Acquisition | Technical Problem Solving
Machine Learning & Data Science
Deep Learning & Representation Learning | Graph Neural Networks | Transfer Learning | Supervised & Unsupervised Learning | Model Evaluation & Validation
Python (PyTorch, scikit-learn, pandas, NumPy, SciPy, Matplotlib, Seaborn, Plotly) | SQL/MySQL | Dash | Git & GitHub | Generative AI Tools
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
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