Abdulmujeeb T. Onawole PhD

Explainable AI Specialist | Computational chemist

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Google Scholar | ORCiD| Scopus| GitHub | LinkedIn

PROFESSIONAL SUMMARY

- **Strong Research Impact**: >1000 citations, h-index 20, 40+ publications, 1 granted US Patent, and deployed interactive prediction tools used by researchers globally
- **Dual Expertise**: 8+ years bridging quantum chemistry (DFT, MD simulations) with modern AI/ML architectures (GNNs, CNNs, generative models)
- **Proven Scale & Deployment:** Screened 1+ million compounds on GPU clusters and deployed production-ready web applications (Hugging Face Spaces), making AI drug discovery accessible to scientists worldwide
- **Open-Source Impact**: Built and deployed antimicrobial prediction tools and XAI frameworks enabling researchers to predict drug activity and understand AI decisions in real-time
- **Translational Research**: Track record of converting complex simulation data into practical solutions for drug discovery and materials science

RESEARCH IMPACT INDICATORS

- **Citations & Productivity:** >1,000 citations and h-index of 20 (Google Scholar); 39 indexed publications and 1 granted US patent
- **Field-Weighted Citation Impact (FWCI):** 1.39 (Scopus) — cited 39% more than the world average for similar publications
- **Publication Quality:** 52.6% of papers in the top 25% most-cited worldwide; 48.6% in top-quartile journals by CiteScore
- **Authorship & Leadership:** 15 first-author papers (39% of indexed output) averaging 25 citations each, with a first-author FWCI of 1.20
- **International Collaboration:** 68.4% of publications co-authored across borders; 95 unique international collaborators
- **Societal Alignment:** Research aligned with UN Sustainable Development Goals 3 (Good Health and Well-Being), 7, 8, 9, and 13, spanning 12 distinct SciVal research topics

EDUCATION

- **PhD, Computational Chemistry** (2026) – *The University of Queensland*, Australia

  Focus: Explainable AI for Antimicrobial Drug Discovery.

- **M.Sc., Chemistry** (2017) – *King Fahd University of Petroleum & Minerals*, Saudi Arabia

  Focus: Computational Chemistry and Molecular Modeling.

- **B.Tech., Pure & Applied Chemistry** (2011) – *Ladoke Akintola University of Technology*. Nigeria

  Focus: Computational Chemistry and Molecular Modeling.

RESEARCH EXPERIENCE

Researcher | Explainable AI & Cheminformatics

Institute for Molecular Bioscience, The University of Queensland | April *2022–Present*

Developed a trustworthy AI system accelerating antimicrobial drug discovery:

- Accelerate drug discovery for the global AMR crisis by developing machine learning models achieving 90%+ accuracy, screening ~ 1M compounds and reducing timelines from years to months.
- Solved the AI "black box" problem by building an explainability framework revealing why predictions succeed or fail, enabling chemists to validate recommendations before expensive laboratory testing
- Established pathogen-selective design rules distinguishing Gram-positive, Gram-negative, and fungal compounds, providing medicinal chemists with actionable strategies for targeted antibiotic design
- Democratized AI drug discovery by deploying an interactive web application enabling any researcher worldwide to predict activity and visualize explanations without coding
- Enabled reproducible research by releasing a complete open-source framework (GitHub/Zenodo) with trained models and datasets, adopted by research teams globally.

Researcher | Computational Chemistry & Molecular Modelling *Gas Processing Center, Qatar University* | December *2017– March 2022*

Gas Processing Center, Qatar University | 2017–2022

- Addressed critical oilfield scale problem where conventional corrosive acid treatments generate toxic hydrogen sulfide (H_2S) gas - a deadly hazard to workers - and cause severe equipment corrosion, disrupting production in oil and gas wells.
- Used computational chemistry (DFT, *ab initio* molecular dynamics) to screen and design green chemical alternatives, validating candidates through experimental testing at high-temperature, high-pressure reservoir conditions before field deployment.
- Computational work led to a **granted US Patent** (US20210108124A1) for an environmentally safe formulation that dissolves scale without generating deadly H_2S while achieving significantly lower corrosion than conventional corrosive acid with inhibitor.

SKILLS

Machine Learning & AI
Graph Neural Networks, CNNs, Ensemble Learning, Generative Models, Explainable AI (Perturbation methods: Substructure masking, Integrated Gradients), PyTorch, scikit-learn

Computational Chemistry
DFT, *Ab Initio* MD, QM/MM, Molecular Docking, Virtual Screening, Gaussian, VASP, Materials Studio

Cheminformatics & Drug Discovery
QSAR Modeling, Molecular Fingerprinting, Structure-Activity Relationships, RDKit

High-Performance Computing
GPU Cluster Deployment, SLURM, Parallel Computing, Large-Scale Virtual Screening (100K-1M+ compounds)

Programming & Data Science
Python, Bash, SQL, pandas, NumPy, Git/GitHub, Docker

AI-assisted workflows

Agentic coding (Claude Code, Codex), literature synthesis, automated analysis pipelines

KEY TECHNICAL PROJECTS

XAI Evaluation Framework for Drug Discovery

Built a systematic four-tier evaluation framework that assesses whether any AI/ML model's explanations are trustworthy and scientifically valid - adaptable across domains by testing: (1) does the model recognize known concepts in the field, (2) can it distinguish context-sensitive differences, (3) do predictions align with explanations, and (4) are results consistent across model variations.

Impact: Developed a framework for evaluating XAI methods to determine if their predictions can be trusted; the framework can be adapted to any field using the four criteria.

Antimicrobial Activity Prediction System

Developed an end-to-end AI pipeline predicting antimicrobial activity and explaining *why* through molecular fragment analysis - deployed as an interactive web application enabling researchers worldwide to test compounds without coding.

Impact: Predicts against *S. aureus*, *E. coli*, *and C. albicans* with 88-95% precision; provides visual fragment attributions guiding medicinal chemists on which modifications improve activity.

Available: https://huggingface.co/spaces/catenate/antimicrobial-xai-predictor

Generative AI Model for Antimicrobial Drug Design

Built a generative model that creates novel antimicrobial drug candidates by identifying effective molecular building blocks from existing data, then systematically combining them to generate 700 new molecules - demonstrating AI can design promising drug leads, not just predict activity of known compounds.

Impact: Generated molecules achieved 40% predicted activity rate, with 99.6% being novel (not present in the training dataset the AI learned from); the system produces pathogen-specific candidates targeting bacteria or fungi selectively.

Polymer Property Prediction with Explainable AI

Built a multi-property prediction system for polymer membranes using graph neural networks, addressing extreme data imbalance (0-89% property coverage) through adaptive loss weighting and confidence-validated explainability.

Impact: Predicts fractional free volume (FFV) for CO_2 separation membranes with 78% of high-confidence predictions achieving ≤5% error; fragment attribution guides rational polymer design

FULL LIST OF PUBLICATIONS

Patents

- **P1.** Ahmed, M., Hussein, I. A., **Onawole, A.**, & Saad, M. (2021). **US 20210108124 A1** – Iron sulphide scale removal from oil and gas wells using green formulation. *United States Patent*.

Journal Articles

- **J39. Onawole, A.**, Blaskovich, MAT, Zuegg, Johannes. (2026). Framework for evaluating explainable AI in antimicrobial drug discovery. *Journal of Cheminformatics*, [Q1]

- **J38.** Friberg, L. I. M., Kavanagh, A., Amado, M., …, **Onawole, A.**, et al. (2025). Organoselenium compounds as an enriched source for the discovery of new antimicrobial agents. *RSC Medicinal Chemistry*, 16(11). [Q1]
- **J37.** Aderinto, S. O., John, T., **Onawole, A.**, Galleh, R. P., & Thomas, J. A. (2024). Iridium(III)-based minor groove binding complexes as DNA photocleavage agents. *Dalton Transactions*. [Q2]
- **J36.** Alli, Y. A., Bamisaye, A., **Onawole, A.**, …, Youssef, K. (2024). Coaxial electrospinning: design, characterization, mechanistic insights and their emerging applications in solar cells. *Nano Energy*, 131, 110203. [Q1]
- **J35.** Alli, Y. A., Oladoye, P. O., **Onawole, A.**, … Philippot, K. (2023). Photocatalysts for CO_2 reduction and computational insights. *Fuel*, 344, 128101. [Q1]
- **J34. Onawole, A.**, Hussein, I. A., Saad, M., Ismail, N., & Nasser, M. S. (2022). Theoretical studies of a silica functionalized acrylamide for calcium scale inhibition. *Polymers*, 14(12). [Q1]
- **J33.** Popoola, S., **Onawole, A.**, Ullah, N., & Al-Saadi, A. (2021). Structural and energetic effect of the intramolecular hydrogen bonding in 4,6-dihaloresorcinols: ab initio calculation, vibrational spectroscopy and molecular docking studies. *Structural Chemistry*, 33(1). [Q3]
- **J32.** Jalab, R., Saad, M., Hussein, I. A., & **Onawole, A.** (2021). Calcite scale inhibition using environmental-friendly amino acid inhibitors: DFT investigation. *ACS Omega*, 6(45). [Q1]
- **J31.** Hamza, A., Shamlooh, M., Hussein, I. A., Nasser, M. S., **Onawole, A.**, et al. (2021). Impact of aluminium acetate particle size on the gelation kinetics of polyacrylamide-based gels: rheological and molecular simulation study. *Canadian Journal of Chemical Engineering*, 100(6), 1169-1177. [Q3]
- **J30. Onawole, A.**, Hussein, I. A., Saad, M., Nimir, H., & Ahmed, M. (2021). Molecular design of novel chemicals for iron sulfide scale removal. *Journal of Chemistry*. [Q2]
- **J29. Onawole, A.**, Nasser, M. S., Hussein, I. A., Al-Marri, M. J., & Aparicio, S. (2021). Theoretical studies of methane adsorption on silica-kaolinite interface for shale reservoir application. *Applied Surface Science*. [Q1]
- **J28.** Ahmed, M., Hussein, I. A., **Onawole, A.**, & Saad, M. (2021). Electrochemical removal of pyrite scale using green formulations. *Scientific Reports*, 11(1). [Q1]
- **J27. Onawole, A.**, Hussein, I. A., Saad, M., Ahmed, M., & Nimir, H. (2021). Computational screening of potential inhibitors of Desulfobacter postgatei for pyrite scale prevention in oil and gas wells. *ACS Omega*, 6(11). [Q1]
- **J26.** Ahmed, M., Hussein, I. A., **Onawole, A.**, & Saad, M. (2020). Pyrite-scale removal using glutamic diacetic acid: a theoretical and experimental investigation. *SPE Production & Operations*. [Q2]
- **J25.** Al Hamad, M., Al-Sobhi, S. A., **Onawole, A.**, … Khraisheh, M. (2020). Density-functional theory investigation of barite scale inhibition using phosphonate and carboxyl-based inhibitors. *ACS Omega*, 5(12). [Q1]
- **J24.** Ahmed, M., Hussein, I. A., **Onawole, A.**, … Mahmoud, M. (2020). Dissolution kinetics of different inorganic oilfield scales in green formulations. *ACS Omega*, 5(11). [Q1]
- **J23.** Ahmed, M., Hussein, I. A., **Onawole, A.**, & Saad, M. (2020). Development of a new borax-based formulation for the removal of pyrite scales. *ACS Omega*, 5(6). [Q1]
- **J22. Onawole, A.**, Sulaiman, K. O., Kolapo, T. U., … Adegoke, R. (2020). COVID-19: CADD to the rescue. *Virus Research*, 286, 198022. [Q2]

- **J21. Onawole, A.**, Hussein, I. A., Carchini, G., Sakhaee-Pour, A., & Berdiyorov, G. (2020). Effect of surface morphology on methane interaction with calcite: a DFT study. *RSC Advances*, 10, 14779-14788. [Q1]
- **J20. Onawole, A.**, Hussein, I. A., Ahmed, M., Saad, M., & Aparicio, S. (2020). Ab initio molecular dynamics of the dissolution of oilfield pyrite scale using borax. *Journal of Molecular Liquids*, 309, 112500. [Q1]
- **J19.** Ahmed, M., Saad, M., Hussein, I. A., **Onawole, A.**, & Mahmoud, M. (2019). Effect of pH on acidic and basic chelating agents used in the removal of iron sulphide scales: a computational study. *Journal of Petroleum Science and Engineering*, 176, 1065-1073. [Q2]
- **J18.** Ahmed, M., Mahmoud, M., Hussein, I. A., **Onawole, A.**, & Saad, M. (2019). Pyrite scale removal using green formulations for oil and gas applications: reaction kinetics. *Energy & Fuels*, 33(4), 3304-3313. [Q1]
- **J17. Onawole, A.**, Hussein, I. A., Sultan, A., Abdel-Azeim, S., Mahmoud, M., & Saad, M. (2019). Molecular and electronic structure elucidation of Fe^{2+}/Fe^{3+}-complexed chelators used in iron sulphide scale removal in oil and gas wells. *Canadian Journal of Chemical Engineering*, 97(1), 386-398. [Q3]
- **J16.** Sulaiman, K. O., **Onawole, A.**, Shuaib, D. T., & Saleh, T. A. (2019). Quantum chemical approach for chemiluminescence characteristics of di-substituted luminol derivatives in polar solvents. *Journal of Molecular Liquids*, 282, 159-168. [Q1]
- **J15.** Asghar, A., Yousuf, M., Mubeen, H., Nazir, R., Haruna, K., **Onawole, A.**, & Rasheed, L. (2019). Synthesis, spectroscopic characterization, molecular docking and theoretical studies of N-(4-aminophenylsulfonyl)-2-(4-isobutylphenyl) propanamide having potential enzyme inhibition applications. *Bioorganic & Medicinal Chemistry*, 27(10), 2235-2247. [Q2]
- **J14.** Sulaiman, K. O., **Onawole, A.**, Faye, O., & Shuaib, D. T. (2019). Understanding the corrosion inhibition of mild steel by selected green compounds using chemical quantum based assessments and molecular dynamics simulations. *Journal of Molecular Liquids*, 277, 285-296. [Q1]
- **J13. Onawole, A.**, Hussein, I. A., Saad, M., & Nimir, H. (2019). Effect of pH on acidic and basic chelating agents used in the removal of iron sulphide scales: a computational study. *Journal of Petroleum Science and Engineering*, 176, 1074-1084. [Q2]
- **J12. Onawole, A.**, Sulaiman, K. O., Kolapo, T. U., … Badmus, S. (2018). Molecular dynamics and combined docking studies for the identification of Zaire Ebola virus inhibitors. *Journal of Biomolecular Structure and Dynamics*, 36(18), 4899-4912. [Q2]
- **J11.** Buijs, W., Hussein, I. A., Mahmoud, M., **Onawole, A.**, & Saad, M. (2018). A molecular modelling study towards the development of H_2S-free removal of iron sulphide scale from oil and gas wells. *Industrial & Engineering Chemistry Research*, 57(26), 8938-8948. [Q1]
- **J10. Onawole, A.**, Popoola, S., Saleh, T. A., & Al-Saadi, A. A. (2018). Silver-loaded graphene as an effective SERS substrate for clotrimazole detection: DFT and spectroscopic studies. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 191, 364-372. [Q2]
- **J9. Onawole, A.**, Halim, M. A., Ullah, N., & Al-Saadi, A. A. (2018). Structural, spectroscopic and docking properties of resorcinol, its –OD isotopomer and dianion derivative: a comparative study. *Structural Chemistry*, 29(3), 855-866. [Q3]
- **J8.** Seliman, A. A. A., Altaf, M., **Onawole, A.**, Al-Saadi, A. A., Ahmad, S., Alhoshani, A., Bhatia, G., & Isab, A. A. (2018). Synthesis, structure and cytotoxicity evaluation of carbene-based gold(I) complexes of selenones. *Inorganica Chimica Acta*, 478, 179-187. [Q3]
- **J7. Onawole, A.**, Al-Ahmadi, A. F., Mary, S. Y., Panicker, C. Y., Ullah, N., Armaković, S., Armaković, S. J., Van Alsenoy, C., & Al-Saadi, A. A. (2017). Conformational, vibrational and DFT studies of a

newly synthesized arylpiperazine-based drug and evaluation of its reactivity towards the human GABA receptor. *Journal of Molecular Structure*, 1144, 356-369. [Q2]

- **J6. Onawole, A.**, Sulaiman, K. O., Kolapo, T. U., & Adegoke, R. (2017). Structure-based virtual screening of the Ebola virus trimeric glycoprotein using consensus scoring. *Computational Biology and Chemistry*, 70, 173-182. [Q2]
- **J5.** Seliman, A. A. A., Altaf, M., **Onawole, A.**, Ahmad, S., Ahmed, M. Y., Al-Saadi, A. A., Altuwaijri, S., Bhatia, G., Singh, J., & Isab, A. A. (2017). Synthesis, X-ray structures and anticancer activity of gold(I)-carbene complexes with selenones as co-ligands and their molecular docking studies with thioredoxin reductase. *Journal of Organometallic Chemistry*, 848, 165-176. [Q3]
- **J4.** Al-Shalalfeh, M. M., **Onawole, A.**, Saleh, T. A., & Al-Saadi, A. A. (2017). Spherical silver nanoparticles as substrates in surface-enhanced Raman spectroscopy for enhanced characterization of ketoconazole. *Materials Science and Engineering C*, 79, 843-851. [Q1]
- **J3.** Saleh, T. A., Al-Shalalfeh, M. M., **Onawole, A.**, & Al-Saadi, A. A. (2017). Ultra-trace detection of methimazole by surface-enhanced Raman spectroscopy using gold substrate. *Vibrational Spectroscopy*, 91, 142-149. [Q3]
- **J2. Onawole, A.**, Sulaiman, K. O., Adegoke, R., & Kolapo, T. U. (2017). Identification of potential inhibitors against the Zika virus using consensus scoring. *Journal of Molecular Graphics and Modelling*, 74, 24-31. [Q2]
- **J1.** Sulaiman, K. O., **Onawole, A.** (2016). Quantum chemical evaluation of the corrosion inhibition of novel aromatic hydrazide derivatives on mild steel in hydrochloric acid. *Computational and Theoretical Chemistry*, 1092, 37-46. [Q2]

Conference Papers, Reports & Preprints

- **R1.** Pratt, M., Samanta, S., McIntyre, L., Luong, Q. H., Erskine, N., & **Onawole, A.** (2023). What is the future of work for multicultural Australia? *Report*.
- **C1. Onawole, A.**, Hussein, I. A., Ahmed, M., & Aparicio, S. (2020). DFT–MD dissolution of oilfield pyrite scale using borax. *International Conference Proceedings*.
- **C2.** Ahmed, M., **Onawole, A.**, Hussein, I. A., & Nimir, H. (2019). Application of DFT in iron sulphide scale removal from oil and gas wells. *Third EAGE WIPIC Workshop: Reservoir Management in Carbonates*.
- **C3.** Ahmed, M., **Onawole, A.**, Hussein, I. A., Saad, M., & Mahmoud, M. (2019). Effect of pH on dissolution of iron sulphide scales using THPS. *SPE International Conference on Oilfield Chemistry*.
- **C4. Onawole, A.**, Sulaiman, K. O., Kolapo, T. U., & Adegoke, R. (2018). Identification of small molecules as antiviral agents in the treatment of Ebola virus disease using consensus scoring. *Poster Presentation*.
- **C5. Onawole, A.**, & Al-Saadi, A. A. (2016). Computational study of the conformations and molecular docking of the anti-fungal drug clotrimazole in aiding drug delivery via nanostructured lipid carriers. *Poster Presentation*.

INVITED TALKS & CONFERENCE PRESENTATIONS

Onawole, A. T. (2025). *Finding Key Building Blocks for Antibiotics with Deep Learning*. Advancing Data Technologies to Corner AMR (ADTCA) 2025 — International Matchmaking Symposium, AMR Insights, 19–20 June 2025 (online). Recording: https://youtu.be/iS2qpQCunu4?t=1828 (presentation begins at 30:28).

PROFESSIONAL AFFILIATIONS & SERVICE

- Member, American Chemical Society (ACS)
- Member, Royal Australian Chemical Institute (RACI)
- Reviewer for chemistry journals including *RSC Advances* and *Chemistry Africa*

AWARDS & SCHOLARHSIPS

- **Research Training Program (RTP) Scholarship** | The University of Queensland, Australia (2022–Present)
  Awarded highly competitive Australian Government scholarship covering full tuition and living stipend for PhD research
- **M.Sc. Graduate Scholarship** | Ministry of Higher Education, Saudi Arabia (2014–2017)
  Full merit-based scholarship covering tuition and stipend for master's studies at King Fahd University of Petroleum & Minerals (KFUPM)

COMMUNITY SERVICE & MENTORSHIP

- **Academic Mentor & Coordinator** | LAUTECH Alumni Network
  Coordinate academic guidance for alumni and mentor undergraduate students from Nigeria on academic writing and global scholarship applications; successfully mentored multiple students who subsequently won fully funded scholarships for graduate studies in the USA and Canada
- **Invited Guest Speaker** | The Grind Path (Educational Series)
  Featured on episode "Navigating Scholarship Opportunities Across Continents" to advise students from low-and-middle-income countries on leveraging education for social mobility
  Video Available

PROFESSIONAL DEVELOPMENT & TRAINING

RASPA Molecular Simulations Workshop | Wrocław University of Science and Technology, Poland (July 1–4, 2019)
Selected for intensive 4-day training on Molecular Dynamics (MD) and Monte Carlo (MC) simulations for adsorption/diffusion in nanoporous materials and ionic liquids; fully funded by Qatar University