Dr. AD Dinga **Wonanke**

Senior Computational Chemist & Research Software Engineer

AI-Driven Materials Discovery | Machine Learning | MOFs | Scientific Python | HPC

Personal

Dominique Akassong Dinga Wonanke
Nationality: Cameroonian
Resident: UK Global Talent

Profession

Postdoc in Computational Chemistry.

Alumni Network

MSCA Fellow
Falling Walls
Lindau Noble Laureate

Contact

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Areas of Expertise

Computational Chemistry
Materials Discovery
Synthesis Prediction
Cheminformatics
Battery Materials
Hydrogen Storage
CO_2 Capture
Graph Neural Network
Large Language Modelling
Data Science

Top Technical Skills

Programming
Python, Bash & NodeJS

AI & LLM
HuggingFace Transformers, PyTorch & PyTorch-goemetric

Data Science
Pandas, Scikit-Learn, NumPy & SciPy

NLP
NLTK, spaCy & RegEx

Web Dev
HTML, CSS & JavaScript

Web Frameworks
Bootstraps, Next.js, React, Django, Flutter

DevOps

Summary

I am a senior computational scientist and research software engineer with 10+ years experience in building AI driven models and production-grade software for materials discovery. Proven track record in deploying machine-learning systems, large-scale simulations and scientific platforms used by researchers and industry. Experienced in leading cross-disciplinary projects from concept to deployment.

- Built a Graph Neural Network (GNN) to predict MOF synthesis conditions directly from 3D crystal structures.
- Applied text mining and NLP techniques to extract synthesis conditions from 40+ peer-reviewed journal articles.
- Curated a structure-synthesis dataset of 40+ MOFs that links experimental conditions to 3D structural representations.

Professional Experience

2026–present

Senior Postdoctoral Fellow
Nottingham Trent University · United Kingdom
Designing machine-learning based predictive models to quantify the impact of isomerism on gas adsorption in porous framework materials. In parallel, I am developing a startup based on a spinout from my MSCA-funded research.

2023–2025

Marie Skłodowska-Curie Postdoctoral Fellow
Technical University of Dresden · Germany
Built and deployed a Graph Neural Network that predicts MOF synthesis conditions directly from 3D structures, enabling data-driven experimental planning and reducing trial-and-error in synthesis workflows. Led large-scale high-throughput simulations on 40,000+ MOFs to screen candidates for energy storage. Secured 15M HPC CPU hours and built production-ready Python and web-based tools for synthesis planning and database exploration. Co-authored publications in JACS and Nature Chemistry and finalist at Falling Walls Lab Berlin.

2021–2023

Postdoctoral Researcher Fellow
Karlsruhe Institute of Technology (KIT) · Germany
Designed scalable data pipelines for curating and standardising 34,000+ MOF structures within the NOMAD repository to improve reproducibility and downstream ML readiness. Developed `mofstructure`, an open-source Python engine for automated framework classification and descriptor extraction and published a curated dataset of 34,000+ geometry-optimized MOFs with interactive search and 3D visualization tools.

2019–2021

Postdoctoral Researcher
Nottingham Trent University · United Kingdom
Led computational materials projects involving large-scale deconstruction of 80,000+ MOF/COF structures into reusable molecular building blocks, integrated into SCM's AuToGraFS software. Performed docking and molecular dynamics simulations, collaborated with experimentalists on PXRD-based structure validation and contributed to materials design for separation technologies. Co-authored eight peer-reviewed publications and delivered Python programming training.

July 2025

Research Visitor
Karlsruhe Institute of Technology (KIT) · Germany
Gained hands-on experimental experience by programming and configuring a robotic platform for layer-by-layer epitaxial growth of γ-cyclodextrin SURMOFs. Conducted vapour diffusion and vapour deposition synthesis and applied advanced characterization techniques including TOF-SIMS, SEM and in-/out-of-plane XRD to optimize film growth.

GitHub, GitLab, SVN, Docker, CI/CD

Platform & OS
HPC, MacOS, Linux, Windows, SLURM

Other
FastAPI, Flask, Flutter, Dart, Rust

Computational Chemistry

Cheminformatics
ASE, Pymatgen, RDKit, Openbabel, PubChem, CSD API

ComChem Software
AMS, Gaussian, QChem, ORCA, CP2K, FHI-AIMS, RASPA, DFTB+, GROMACS, LAMMPS

Selected Resources
cheminteraction.com
mofbattery.com
FAIR-MOF database
mofstructure
fairmofsyncondition
Docking

Professional Profile
GitHub
LinkedIn
ORCID
Google Scholar

Pitches & Media
Pitch Video Falling Walls Lab Berlin
Determining Carbonate Content in Antacids
Acids and Bases

References

Dr. Deborah Crittenden
PhD Supervisor
deborah.crittenden@canterbury.ac.nz

Dr. Matthew Addicoat
Postdoc Supervisor
matthew.addicoat@ntu.ac.uk

Degrees

2015–2019 **PhD in Chemistry**
University of Canterbury · New Zealand

2011–2014 **M.Sc. Chemistry**
University of Dschang · Cameroon

2008–2011 **B.Sc. Chemistry**
University of Dschang · Cameroon

Programming

Python
Bash
PyTorch
Transformers
HTML, CSS
JavaScript

Additional Professional Experience

2020–present **Scientific Software Developer**
Software for Chemistry & Materials (SCM · Remote / Europe
Maintain and extend the AuToGraFS scientific software package by contributing new code modules, refactoring core components, implementing unit tests and authoring technical documentation and tutorials for annual releases.

2016–2019 **Chemistry Laboratory Supervisor**
University of Canterbury · New Zealand
Led undergraduate chemistry laboratories by delivering pre-lab instruction, supervising experiments, enforcing safety protocols and assessing reports. Developed instructional video resources still used for student induction.

2014–2015 **Chemistry Teacher**
Full Gospel High School · Cameroon
Delivered chemistry lessons across secondary and pre-university levels, organized targeted revision programs for national examinations and supported academic administration through digital record management.

Certificates & Grants

2025 74th Lindau Nobel Laureate Meeting
2024 Finalist at Falling Walls Berlin
2024 MSCA Developing Talents Award
2023 Marie Skłodowska-Curie Postdoctoral Fellowship
2020 HPC-Europa3 Grant

Review Activities

- Nature Communications
- Journal of Chemical Information
- Materials Communication
- Langmuir

Languages

English	C2	Mother tongue
French	C2	● ● ● ●
German	A1	● ● ● ●

Volunteering

2016-present Science outreach activities
2021 Mentor at Cara Fellowship Program
2020 – 2024 AgeUK Telephone Befriender Program

Publication

I have published extensively in leading journals, including Nature Chemistry, Nature Communications and JACS. I also have a first-author manuscript currently under review at Nature Computational Science. A complete list of my publications are available on my Google Scholar.

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