Anthony Onwuli

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Location: London, UK

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Education

2020–2024 **PhD in Materials**, Imperial College London, UK.

- *'Rapid computational screening of materials for energy storage'*
- Supervised by Aron Walsh and Keith T. Butler (QMUL/UCL).
- Adapting natural language processing techniques to create ionic representations for applications in property prediction and automated doping suggestions.
- Developing software for analysis and visualisation of high dimensional elemental and ionic representations.
- Designing and implementing workflows for high throughput density functional theory calculations and molecular dynamics simulations for finding new solid state electrolytes.
- Expected submission March 2024

2016–2020 **MEng in Materials Science and Engineering**, Imperial College London, UK.

- First class honours.
- Final year project: *'Rapid structure prediction using structural analogy'*.

Supervision and Teaching Experience

2021–2022 **Supervisor**, Imperial College London, UK.

- Supervised two MSc students on a project on applying element representations to crystal structure prediction via structure substitutions.
- Assisted and co-supervised a UROP student on a project on applying unsupervised machine learning techniques to phonon data to discover solid electrolytes.
- Web scraped data to provide a repository for the UROP project. GitHub: WMD-Group/phonondb

2021–Present **Graduate Teaching Assistant**, Imperial College London, UK.

- Developing Jupyter Notebook teaching materials for new course on machine learning for materials science for master's students.
- Delivered workshops for introduction to python courses for first year materials science undergraduates.
- Guided second year materials science undergraduates through workshops on machine learning using python.

Open Source Research Software

2022–Present **ElementEmbeddings** | GitHub: WMD-Group/ElementEmbeddings
Python package to analyse high-dimensional representations of the chemical elements using different statistical measures
Role: Creator and sole developer

2019–Present **SMACT** | GitHub: WMD-Group/SMACT
Python package to aid materials design and informatics
Role: Lead maintainer, developer, GitHub CI/CD setup

Presentations

Talks

2023 **A. Onwuli**, A.V. Hegde, K. Nguyen, K. T. Butler, A. Walsh. **A periodic table for the machine learning era** *TYC Student Day, University College London, UK*.

2023 **A. Onwuli**, A. M. Ganose, A. Aguadero, A. Walsh, I. Seymour. **Materials design of quaternary sodium halide electrolytes** *Department of Materials Postgraduate Research Day, Imperial College London, UK*.

2023 **A. Onwuli**, A.V. Hegde, K. Nguyen, K. T. Butler, A. Walsh. **Rapid structure prediction** *Machine Learning for Materials: Data-driven materials design (2.0), Imperial College London UK*.

Posters

2023 **A. Onwuli**, A.V. Hegde, K. Nguyen, K. T. Butler, A. Walsh. **Element similarity in high-dimensional materials representations** *CECAM Crystal Structure Prediction workshop, Liverpool, UK*.

2023 **A. Onwuli**, A. M. Ganose, A. Aguadero, A. Walsh, I. Seymour. **Materials design of quaternary sodium halide electrolytes** *RSC MC16, Dublin, Ireland*.

2022 **A. Onwuli**, K. T. Butler, A. Walsh. **Exploration of the oxide garnet search space** *Psi-K 2022, Lausanne, Switzerland*.

2022 **A. Onwuli**, K. T. Butler, A. Walsh. **Exploration of the oxide garnet search space** *CAMD Summer School: Electronic Structure Theory and Materials Design, Helsingor, Denmark*.

Publications

2023 **A. Onwuli**, A. M. Ganose, A. Aguadero, A. Walsh, I. Seymour. *Materials design of quaternary sodium halide electrolytes*, in preparation.

2023 **A. Onwuli**, A.V. Hegde, K. Nguyen, K. T. Butler, A. Walsh. *Element similarity in high-dimensional materials representations*,
Digital Discovery DOI:10.1039/D3DD00121K ArXiv: 10.48550/arXiv.2307.00784

Memberships and Committees

2020–Present **Department of Materials Graduate Society Committee**, Imperial College London, UK.
Role: Cohort representative

- Organised annual postgraduate research days between 2021-2023 including organising speakers, poster sessions and social events.
- Handled PhD student feedback on issues surrounding supervising MSc/MEng student which led to an organised workshop for PhD students on supervising and meetings with project coordinators.

Skills

Programming	Preferred languages: `Python`, other languages: `Bash`, `LaTeX`.
Electronic Structure	Intermediate user of `VASP`.
Materials Informatics	Intermediate user of materials informatics packages including `matminer` and `pymatgen`.
Big Data	Frequent user of database, data mining, web scraping, machine learning and workflow management tools including `MongoDB`, `Pandas`, `Atomate2`, `Fireworks`, `scikit-learn` and `TensorFlow`.

Other	User of `Git` version control, `GitHub` CI/CD, Slurm and SGE job scheduling on high performance computing systems, Mac, Linux and Windows operating systems.