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Location: London, UK

Education

- 2020–2024 **PhD in Materials**, Imperial College London, UK.
- *'Rapid computational screening of materials for energy storage'*
 - Carrying out a project under the supervision of Aron Walsh and Keith Butler (UCL) on computational screening of inorganic materials for solid state electrolytes.
 - Developing software for analysis and visualisation of high dimensional elemental and ionic representations.
 - Applying machine learning techniques to predict the ionic conductivity of materials.
 - 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.
- Day to day supervision of two MSc students on a project on applying element representations to crystal structure prediction via structure substitutions.
 - Day to day co-supervision of an undergraduate 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](https://github.com/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.
 - Delivered workshops for machine learning using python for second year materials science undergraduates.

Open Source Research Software

- 2022–Present **ElementEmbeddings** |  GitHub: [WMD-Group/ElementEmbeddings](https://github.com/WMD-Group/ElementEmbeddings)
Python package to interact with high-dimensional representations of the chemical elements
Role: Creator and sole developer
- 2019–Present **SMACT** |  GitHub: [WMD-Group/SMACT](https://github.com/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, London UK*.
- 2023 **A. Onwuli**, A. M. Ganose, A. Aguiadero, A. Walsh, I. Seymour. **Materials design of quaternary sodium halide electrolytes** *Department of Materials Postgraduate Research Day, 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), 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. Aguiadero, 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. Aguiadero, A. Walsh, I. Seymour. *Materials design of quaternary sodium halide electrolytes*, in preparation (2023).
- 2023 **A. Onwuli**, A.V. Hegde, K. Nguyen, K. T. Butler, A. Walsh. *Element similarity in high-dimensional materials representations*,  ArXiv: [10.48550/arXiv.2307.00784](https://arxiv.org/abs/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.
 - Represented the views of the postgraduate students to the department.
 - Chaired meetings of the committee in 2023.

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.