




Education and Research Experience

- 2020–2024 **PhD in Materials Research**, Imperial College London, UK.
- *'Rapid computational screening of materials for energy storage applications'*
 - Supervised by Aron Walsh and Keith T. Butler (UCL).
 - Funded by a UKRI EPSRC studentship.
 - Adapted natural language processing techniques to create ionic representations for applications in property prediction and automated doping suggestions.
 - Developed software for analysis and visualisation of high dimensional elemental and ionic representations.
 - Designed and implemented workflows for high throughput density functional theory calculations and molecular dynamics simulations for finding new solid state electrolytes.
 - Submitted in 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](https://github.com/WMD-Group/phonondb)
- 2021–2024 **Graduate Teaching Assistant**, Imperial College London, UK.
- Developed 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](https://github.com/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](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. M. Ganose, A. Aguadero, A. Walsh, I. Seymour. **Materials design of quaternary sodium halide electrolytes** *RSC SSCG Christmas Meeting, Edinburgh, UK.*
- 2023 **A. Onwuli**, A. M. Ganose, A. Aguadero, A. Walsh, I. Seymour. **Materials design of quaternary sodium halide electrolytes** *2023 Fall MRS Meeting, Boston MA, USA.*
- 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.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.*

Publications

- 2024 H. Park, **A. Onwuli**, K. T. Butler, A. Walsh. *Mapping inorganic crystal chemical space* Faraday Discussions DOI:[10.1039/D4FD00063C](https://doi.org/10.1039/D4FD00063C)
- 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](https://doi.org/10.1039/D3DD00121K)

Memberships and Committees

- 2020–2024 **Department of Materials Graduate Society Committee**, Imperial College London, UK.
Role: Cohort representative
- Organised annual postgraduate research days between 2021–2024 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.