




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](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.
 - 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.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. Aguiadero, 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. 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 **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.
 - 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

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| 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. |