Dr. Peter John Hatton

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Personal Statement

I am an accomplished **Mathematical Modeller** with extensive and diverse experience in **computational modelling of complex systems**, complemented by a strong record of publishing **high-quality science**. My strengths lie in my robust **mathematical and computational background** as well as my passion for conducting impactful, **cutting-edge science** with sustainable and environmentally conscious applications.

Employment History

Mar 2024 – Present
Guest Scientist, *Los Alamos National Lab, Los Alamos, NM, USA.*
Collaborators: Dr. B.P. Uberuaga, Dr. D. Perez, Dr. T. Frolov and Prof. B. Wirth
Developing a massively parallel, multi-fidelity workflow for approximating defect diffusion tensors in chemically complex materials, integrating atomistic data with machine learning and Monte Carlo algorithms.
Using state-of-the-art molecular modelling techniques coupled with quantum particle simulation to study the microstructural evolution of tungsten under energetic particle bombardment in fusion reactor conditions, integrating large-scale thermodynamic models to predict macroscopic material evolution.

Mar 2021 – Mar 2024
Postdoctoral Researcher, *Los Alamos National Lab, Los Alamos, NM, USA.*
Mentors: Dr. B.P. Uberuaga and Dr. D. Perez.
Utilised atomistic modelling, integrated with higher-length-scale thermodynamic models and experimental measurements through a multi-scale modelling framework, to examine defect kinetics in complex oxide materials under extreme conditions. Primarily focused on projects related to material corrosion and radiation in fission reactors. Led a multi-fidelity project to develop uncertainty quantification methodologies for machine-learned interatomic potential data, benchmarking against quantum-accurate baselines.

Nov 2020 – Mar 2021
Postdoctoral Researcher, *Loughborough University, Loughborough, UK.*
Mentors: Prof. R. Smith and Prof. P. Goddard.
Utilised advanced modelling techniques across various length and time scales to elucidate the previously misunderstood mechanisms in the manufacturing processes of CdTe solar cells. This work led to refinements in manufacturing, resulting in cost reductions and increased efficiency. Mentored PhD students and contributed to the teaching and assessment of undergraduate mathematics courses.

Education

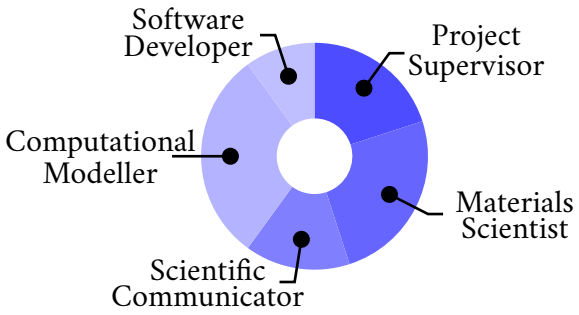
Oct 2017 – Nov 2020
Ph.D., Mathematical Modelling *Loughborough University, Loughborough, UK.*
Supervisors: Prof. R. Smith and Prof. P. Goddard.
Thesis title: Gas Bubbles and Atomic Diffusion Mechanisms in CdTe Solar Cells.

Oct 2016 – Jul 2017
Masters Degree in Mathematics. *Loughborough University, Loughborough, UK.*
First Class Honours.
Dissertation title: The Markov Equation and the Most Irrational Number.

Oct 2012 – Jul 2016
BSc in Mathematics. *Loughborough University, Loughborough, UK.*
First Class Honours.

Skills & Attributes

Professional Attributes



Core Competencies

Atomistic Simulation (Classical/Quantum)
Accelerated Molecular Dynamics
Parallel Computing
Multi-Scale Modelling
Machine Learning
Monte Carlo Methods
Python/C++
Uncertainty Quantification
Training & Development
Data Visualization
Unix/Linux Systems

Publication Highlights

- **Hatton, P.**, Perez, D., Frolov, T., & Uberuaga, B. P. (2024). He Bubble-induced Phase Transformation of W Grain Boundaries Revealed by Accelerated Molecular Dynamics. *Acta Materialia*, 119821. https://doi.org/10.1016/j.actamat.2024.119821
- **Hatton, P.**, & Uberuaga, B. P. (2023). Short Range Order in Disordered Spinels and the Impact on Cation Vacancy Transport. *Journal of Materials Chemistry A*, *11*(7), 3471–3480. https://doi.org/10.1039/D2TA06102C
- Kaspar, T. C., **Hatton, P.**, Yano, K. H., Taylor, S. D., Spurgeon, S. R., Uberuaga, B. P., & Schreiber, D. K. (2022). Adatom-Driven Oxygen Intermixing during the Deposition of Oxide Thin Films by Molecular Beam Epitaxy. *Nano Letters*. https://doi.org/10.1021/acs.nanolett.2c01678
- **Hatton, P.**, Watts, M., Abbas, A., Walls, J. M., Smith, R., & Goddard, P. (2021). Chlorine Activated Stacking Fault Removal Mechanism in Thin Film CdTe Solar Cells: The Missing Piece. *Nature Communications*, *12*. https://doi.org/10.1038/s41467-021-25063-y
- Watts, M. J., **Hatton, P.**, Smith, R., Fiducia, T., Abbas, A., Greenhalgh, R., Walls, J. M., & Goddard, P. (2021). Chlorine Passivation of Grain Boundaries in Cadmium Telluride Solar Cells. *Physical Review Materials*, *5*. https://doi.org/10.1103/PhysRevMaterials.5.035403

A complete list of publications is available on Google Scholar

Recent Technical Seminars

Nov - 2023 — **(Invited) Center for Non-linear Studies**, *Exploiting High Performance Computing Resources to drive Time-Parallelized Molecular Dynamics in a GPU-Dominated World*, Los Alamos, NM, USA

Mar - 2023 — **(Invited) New Mathematics for the Exascale: Applications to Materials Science**, *3 Month Program*, UCLA, Los Angeles, CA, USA.

The Minerals, Metals & Materials Society (TMS), *Short Range Order in Disordered Spinel and the Impact on Cation Vacancy Transport*, San Diego, CA, USA.

Oct - 2022 — **(Invited) Advances in PV Materials Modelling Webinar**, *Atomistic Modelling of Inert Gas Bubble Growth in Magnetron Sputtered Thin Film CdTe*, Online.

The 10th International Conference on Multiscale Materials Modeling, *Long Time-Scale Molecular Dynamics Modeling of He Bubble Growth at W Grain Boundaries*, Baltimore, MD, USA.

References

Available on request