Dr. Peter John Hatton

pete.hatton21@gmail.com https://petehatton.github.io +44(0)7547 153361
https://orcid.org/0000-0002-2914-2200 https://github.com/PeteHatton

Personal Statement

I am an accomplished materials scientist with extensive and varied experience in computational modeling of materials, complemented by a strong track 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 focused on sustainable and environmentally conscious applications.

Employment History

Mar 2024 – Present
Guest Scientist, *Los Alamos National Lab, Los Alamos, NM, USA.*
Active collaborators: Dr. B.P. Uberuaga, Dr. D. Perez, Dr. T. Frolov, Prof. P.P. Dholabhai and Prof. B. Wirth
Developing a massively-parallel automated workflow for approximating diffusion tensors of defects in High Entropy Alloys with a focus on exploiting exascale computing resources by integrating with machine-learning and kinetic Monte Carlo algorithms. Using accelerated molecular dynamics to study the microstructural evolution of Tungsten under energetic particle bombardment in fusion reactor conditions with integration into mesoscale thermodynamic models for predicting 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.
Using atomistic modelling, integrated with higher length scale thermodynamic models through a multi-scale modelling framework, to examine the kinetics of defects in complex material environments under extreme conditions. Mainly involved in projects concerning materials in the extreme environments of Fusion and Fission reactors studying microstructural damage evolution.

Nov 2020 – Mar 2021
Postdoctoral Researcher, *Loughborough University, Loughborough, UK.*
Mentors: Prof. R. Smith and Prof. P. Goddard.
I employed advanced modelling techniques at various length and time-scales to elucidate the long misunderstood mechanisms behind the manufacturing processes of CdTe solar cells. This insight increased understanding of these processes in the community and directly improved the efficiency and quality of cell production with our experimental collaborators.

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.

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.**, Hatton, M., Perez, D., & Uberuaga, B. P. (2022). The Importance of Long-Timescale Simulations for Driven Systems: An Example of He Bubble Growth at a W GB. *MRS Communications*, 1–8. https://doi.org/10.1002/adem.202201788
- **Hatton, P.**, Perez, D., & Uberuaga, B. P. (2022). Be Surface Structures on W(110) and W(211): A DFT Study. *Acta Materialia*, 118012. https://doi.org/10.1016/j.actamat.2022.11801
- **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
- **Hatton, P.**, Abbas, A., Kaminski, P., Yilmaz, S., Watts, M., Walls, J. M., Goddard, P., & Smith, R. (2020). Inert Gas Bubble Formation in Magnetron Sputtered Thin Film CdTe Solar Cells. *Proceedings of the Royal Society A*, *476*. https://doi.org/10.1098/rspa.2020.0056

A complete list of publications is available on Google Scholar

Recent Technical Talks

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 **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