

# Lewis A. D. Irvine

Doctoral Researcher in New and Sustainable Photovoltaics

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## Education and Experience

### **PhD in New and Sustainable Photovoltaics (Oct 2017 – Jan 2022)**

Department of Physics, University of Bath, United Kingdom

Thesis title: *Charge-carrier dynamics in lead-halide perovskites*

Supervisors: Prof Alison Walker, Dr Matthew Wolf, Dr Benjamin Morgan

- Lead developer of BoltMC, a Monte Carlo particle-based simulation package designed to solve the Boltzmann transport equation to compute charge transport properties in halide perovskite solar cells. Developed in collaboration with Department of Mathematics, University of Bath using the PPMD performance portable framework to write scalable software with a Python-based interface. The focus of my thesis is the understanding of the Fröhlich interaction between electrons and phonons in halide perovskites, and the accurate calculation of mobilities and hot carrier cooling times using the code that I developed.
- Collaboration with ultrafast spectroscopists at Technical University Munich (Deschler group) to support transient measurements of hot carrier thermalisation and cooling in perovskites.
- Co-supervision of four final year MPhys student projects and training of one PhD student, all using and extending BoltMC to explore aspects of charge carrier dynamics in lead-halide perovskites and other semiconductors.
- Experience with drift-diffusion modelling of perovskite solar cells through co-supervision of two BSc final year students, with device fabrication and impedance spectroscopy support from Petra Cameron group, Department of Chemistry, University of Bath
- Extensive training from EPSRC Centre for Doctoral Training in New and Sustainable Photovoltaics (CDT-PV) including fabrication of perovskite solar cells, advanced characterisation techniques, photovoltaic device physics and entrepreneurial skills. Access to a network across seven leading UK universities in PV research.

### **MPhys Research Placement (Jun – Dec 2016)**

JET Integrated Modelling Group, UK Atomic Energy Authority, Oxfordshire, United Kingdom

Title: *Plasma core transport modelling and power extrapolation in JET using JETTO-TGLF*

Supervisors: Dr Colin Roach, Dr Gabor Szepesi

- Assessed the validity of the trapped gyro-Landau-fluid (TGLF) quasilinear gyrokinetic transport model for plasmas in nuclear fusion tokamaks. This required modelling plasma core density and temperature profiles for the Joint European Torus (JET) using the JETTO suite of integrated modelling codes, then comparing with alternative transport models and JET pulse data.

### **MPhys Physics with Research Placement (Sep 2013 – Jul 2017)**

University of Bath, United Kingdom

First Class (Hons)

**Chipping Campden School, Gloucestershire, United Kingdom (Feb 2010 – Jun 2013)**

**Lesmahagow High School, South Lanarkshire, United Kingdom (Aug 2007 – Jan 2010)**

A-Levels in Physics, Mathematics, Geography, AS-Level Chemistry, 11 GCSE's

## Computational Skills

- Languages: Python, C++, C, some MATLAB
- Adherence to software best practices including version control, unit testing and automatic documentation using CI/CD tools
- Data analysis and visualisation using numpy / scipy / matplotlib libraries
- Experience with OpenMP parallelisation, code generation and domain specific languages
- Familiarity with Python debugging and profiling tools
- Experience running large integrated modelling codes on HPC facilities
- Proficient in the UNIX operating system, Microsoft Office and LaTeX
- Graduate Teaching Assistant roles in undergraduate physics courses, including Programming Skills (fundamental programming concepts in C) and Computational Physics (advanced computational skills and simulation techniques in C++ and Python)

## Publications

*Quantifying polaronic effects on charge-carrier scattering and mobility in lead-halide perovskites*

**L. A. D. Irvine**, A. B. Walker and M. J. Wolf  
*Phys. Rev. B* **103** L220305 (2021)  
DOI: 10.1103/PhysRevB.103.L220305

*Next steps in the footprint project: A feasibility study of installing solar panels on Bath Abbey*  
M. J. Smiles, A. M. Law, A. N. Urwick, L. Thomas, **L. A. D. Irvine**, M. T. Pilot, A. R. Bowman and A. B. Walker  
Accepted in *Energy Science & Engineering*

*Assessing the effects of multiphonon scattering in lead-halide perovskites*  
**L. A. D. Irvine**, J. Lerpinière, A. B. Walker and M. J. Wolf  
In preparation

## Presented Work (Highlights)

(Aural) *Quantifying polaronic effects on charge-carrier scattering and mobility in lead-halide perovskites*  
APS March Meeting, 15 – 19 Mar 2021, Online

(Aural) *Hot carriers in lead-halide perovskites*  
University of Bath Physics PhD Conference, 08 Sep 2020, Online

(Poster) *Charge carrier transport in MAPbI<sub>3</sub>: quasi-free electrons vs. polarons*  
RSC Next Generation Materials for Solar Photovoltaics, 15 Jan 2020, London, United Kingdom

(Poster) *Charge carrier transport in MAPbI<sub>3</sub>: quasi-free electrons vs. polarons*  
PSCO 2019, 30 Sep – 02 Oct 2019, Lausanne, Switzerland

(Aural) *Quantifying the influence of polaronic behaviour on charge transport in MAPbI<sub>3</sub>*  
CDT-PV Showcase, 09 – 12 Sep 2019, University of Bath, United Kingdom

(Poster) *Charge carrier transport in MAPbI<sub>3</sub>: quasi-free electrons vs. polarons*  
Perovskite Solar Cell and Optoelectronics Day, 27 Jun 2019, Oxford, United Kingdom

## Summer Schools and Workshops Attended

*EPSRC Centre for Doctoral Training in New and Sustainable Photovoltaics Showcase*  
31 Oct – 02 Sep 2021, University of Sheffield; 09 – 12 Sep 2019, University of Bath;  
07 – 08 Nov 2018, University of Liverpool; 08 – 09 Nov 2017, University of Liverpool

*VASP Workshop: Electronic Structure Modelling Relevant to Surface and Interface Science*  
22 – 23 Oct 2019, Chester, United Kingdom

*CCP5 Summer School 2018*  
08 – 17 Jul 2018, Lancaster University, United Kingdom

*53<sup>rd</sup> Culham Plasma Physics Summer School*  
18 – 29 Jul 2016, UK Atomic Energy Authority, Oxfordshire United Kingdom

## Other Roles and Achievements

### **City Coordinator, Pint of Science (Sep 2019 – Aug 2021)**

Organised the Bath branch of Pint of Science, an international science festival that engages communities with local researchers in a relaxed, hospitable environment. Recruited a diverse team of volunteers, oversaw training of team and speakers, and liaised with venues and budget holders. Rapidly rescheduled and moved the 2020 festival to an online platform, then coordinated Bath's contribution to the expanded 2021 online festival. Demonstrated excellent leadership and organisational skills under pressure while maintaining a team focused work ethic.

### **University of Bath Outreach (Oct 2019 – Mar 2020)**

Assisted with Department of Physics primary school outreach workshops coordinated by Prof Ventsislav Valev. Winner of Vice-Chancellor's Award for Public Engagement with Research.

### **Trustee, Holy Trinity Combe Down Parochial Church Council (Apr 2018 – Apr 2021)**

A position of responsibility in a medium-sized charity, making and approving budgetary and staffing decisions.

### **Bath City Pastors (Mar 2018 – Nov 2021)**

Supporting the homeless and assisting vulnerable members of the community.

### **Volunteer Marshal (Jan – Nov 2021)**

Volunteering twice monthly at the COVID-19 Large Vaccination Centre at Bath Racecourse.

### **Music**

Clarinet (Grade 8 Jazz), piano (Grade 3).

### **Sport**

Completed the 2020 Virtual London Marathon, raising over £2,000 for a local charity, as well as the 2018, 2019 and 2020 Bath Half Marathons.

## References

**Prof Alison Walker**  
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University of Bath  
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**Dr Matthew Wolf**  
Institute of Physical Chemistry  
RWTH Aachen University  
Email: wolf@pc.rwth-aachen.de