PhD advert template – 2022 entry

Supervisor name/s	Prof Alison Walker
Email contact	a.b.walker@bath.ac.uk
Department	Physics
Title of project	Understanding charge carrier transport in metal-halide perovskite solar cells
Preferred start date	Monday 3 October 2022
Overview of the research Max 350 words (do not include scientific characters or pictures)	Metal–halide perovskites with their distinctive structure have shown great potential as a disruptive solar cell technology due high performance and low production costs [1]. Despite the meteoric rise of this technology, a fundamental understanding of why perovskites make such good photovoltaic materials is missing. This understanding will come from a detailed picture of the underlying physics and is essential to improve cell performance and stability. Perovskite materials are promising for hot carrier solar cells that utilizes the excess thermal energy of photo-excited carriers to generate electric power. Unlike conventional solar cells, hot carrier cells inhibit ultrafast cooling processes, and their thermalization and extraction remain largely unexplored [2]. This project will study hot carrier dynamics in perovskites using theoretical and computational methods. The student will adapt and extend state-of-the-art computational codes developed by the group which use random walk Monte Carlo (at the mesoscale, 10-100 nm) [3] and drift diffusion models (at the continuum scale, exceeding 100 nm) [4] with parameters obtained from atomistic calculations as input. Our Monte Carlo code is unique in being able to study mesoscale phenomena which affect perovskites due to their heterogeneity at multiple length scales [5] We are modelling spectroscopy measurements from a group in Germany and have excellent contacts with other perovskite groups through the Centre for Doctoral Training in New and Sustainable Photovoltaics and the Horizon2020 Innovative Training Network, Maestro MAking pErovskiteS TRuly exploitable, both directed by Walker [6[. There is also a longstanding collaboration with the experimental group of Prof Petra Cameron in Bath Chemistry. The student will gain transferable skills in coding with Python, C, electronic structure packages, data analysis and working across disciplines and with experimental groups. He/she will have access to the HPC clusters available at Bath and 8 servers dedicated to Walker's group. They will benefit from soft skills postgraduate training and take part in conferences and summer schools. Outreach activities and contributions to social media will provide presentation skills and visibility to this project.
References (optional) If required, you may include a small number of recent publications	1. https://undecidedmf.com/episodes/perovskite-solar-cells-may-be-the-future-of-energy 2. I Ahmed et al Light Sci Appl **10**, 174 (2021) DOI s41377-021-00609-3 3. M J Wolf, L A D Irvine, AB Walker Phys Rev B **103**, L220305 (2020) DOI 10.1103/PhysRevB.103.L220305 4. J M Cave et al *J. Applied Phys*. **128**, 184501 (2020) DOI 10.1063/5.0021849 5. E M Tennyson et al Nat Rev Mater **4**, 573 (2019) DOI 10.1038/s41578-019-0125-0 6. https://people.bath.ac.uk/pysabw/.
Industrial partner (if any) Give details of any industrial collaboration in the project	
Candidate requirements Give details of academic background/experience required	Applicants must have obtained, or be about to obtain, a First or Upper Second Class UK Honours degree, or the equivalent qualifications gained outside the UK, in any of physics, chemistry, mathematics or natural sciences and have a strong interest in coding
Application deadline	Applications considered at any time, but preferably before Sunday 13 March 2022

Funding eligibility *Note from the Doctoral College: this information is based on current expectations and we will ensure that the text reflects the latest government guidance at the time of advertising.*	This project is for students able to self-fund their PhD studies only.
Programme Please select ONE	☐ PhD in Biochemistry ☐ PhD in Biology ☐ PhD in Chemistry ☐ PhD in Computer Science ☐ PhD in Mathematics ☐ PhD in Statistics ☐ PhD in Pharmacy & Pharmacology ☒ PhD in Physics

Discipline and subject (taken from FindAPhd)

Insert an X in the box next to all that apply (max 10)

Biological & Medical Sciences		Chemical Sciences		Physical sciences		Engineering
	Agricultural Sciences		Agricultural Chemistry		Applied Physics		Acoustics
	Biochemistry		Analytical Chemistry		Astrophysics		Aeronautical, Maritime and Transport Engineering
	Bioinformatics		Biochemistry		Atmospheric Physics		Biomedical Engineering
	Biomedical Engineering		Chemical Engineering		Atomic Physics		Chemical Engineering
	Biophysics		Chemical Toxicology		Biophysics		Civil & Structural Engineering
	Biotechnology	x	Computational Chemistry	x	Condensed Matter Physics	x	Electrical & Electronic
	Botany / Plant Science		Electrochemistry		Fluid Dynamics	x	Energy
	Cancer / Oncology		Environmental Chemistry		Geophysics		Environmental Engineering
	Cardiovascular Science		Food Chemistry		Low-temperature Physics		Manufacturing
	Cell Biology / Development		Geochemistry	x	Materials Science		Materials Science
	Ecology & Conservation		Inorganic Chemistry		Medical / Biomedical Physics		Mechanical Engineering
	Endocrinology		Macromolecular Chemistry		Metrology	x	Nanotechnology
	Evolution		Materials Science		Nuclear Physics		Nuclear Engineering
	Food Science / Nutrition		Organic Chemistry		Optical Physics		Petrochemical Engineering
	Forensic Science		Pharmaceutical / Medicinal Chemistry		Particle Physics		Semiconductors
	Genetics	x	Physical Chemistry		Plasma Physics		Software Engineering
	Immunology		Synthetic Chemistry		Quantum Physics		Telecommunications
	Marine Biology	**Earth Sciences**			Radiation	**Social Science & Health**	
	Medical/Biomedical Physics		Agronomy & Soil Science	x	Semiconductors		Anthropology
	Medical / Clinical Science		Atmospheric Physics	x	Solid state Physics		Architecture & the Built Environment
	Medical Imaging		Climatology & Climate Change	x	Theoretical Physics		Education
	Microbiology		Ecology & Conservation	**Maths & Computing**			Gender & Sexuality
	Molecular Biology		Ecotoxicology & Pollution		AI & Machine Learning		Health Sciences
	Neuroscience / Neurology		Environmental Chemistry		Applied Mathematics		Psychology
	Obstetrics, Gynaecology & Reproduction		Environmental Engineering		Bioinformatics		Public Health & Epidemiology
	Ophthalmology & Visual Science		Environmental Science		Computational Chemistry		Social Work, Social Policy & Administration
	Palaeobiology		Geochemistry		Computer Science & IT		Sociology
	Parasitology		Geography		Data Analysis		
	Pathology		Geology		Information Science		
	Pharmacology / Toxicology		Geophysics		Mathematics		
	Pharmacy / Pharmaceutics		Hydrology		Operational Research		
	Physiology & Sports Science		Meteorology		Software Engineering		
	Psychology & Psychiatry		Oceanography		Statistics		
	Public Health & Epidemiology		Palaeontology				
	Structural Biology						
	Virology						
	Zoology/Animal Science						