

Emerging materials for optoelectronics applications

1-3 July 2026 | Edinburgh, UK



Faraday Discussions

Wednesday 1 July 2026 (all timings are BST)

11:00	Registration and refreshments
12:00	Lunch
12:45	Welcome and introductions Mirjana Dimitrievska and David Fermin, <i>Co-Chairs of Scientific Committee</i>
12:55	Outline of Discussion format Hannah Hamilton and Shruti Karnik, <i>Royal Society of Chemistry Publishing Editors</i>
13:00	Introductory lecture – Spiers Memorial lecture (Session chair: David Fermin) Robert Martin <i>University of Strathclyde, UK</i>
	Session 1: Computational design and modelling of next generation optoelectronic materials (Session chairs: Andrea Crovetto and Lucy Whalley)
14:00	Octahedral Tilting in Halide Double Perovskites: Disentangling Lone-Pair Chemistry and Geometric Effects Julia Wiktor <i>Chalmers University of Technology, Sweden</i>
14:05	Machine Learning Modeling of Temperature-Dependent Optoelectronic Properties of Anharmonic Solid Solutions Claudio Cazorla <i>Universitat Politècnica de Catalunya, Spain</i>
14:10	Hydroxylation-Driven Type-I to Type-II Band Alignment Transition in WS₂/m-plane ZnO Heterostructures Dedi Sutarma <i>University of Duisburg-Essen, Germany</i>
14:15	Discussion
15:30	Refreshments
16:00	On the possibility of hybrid chalcogenide perovskite photovoltaics Alexander M Ganose <i>Imperial College London, UK</i>
16:05	First Principle calculations of the internal conversion and intersystem crossing rates of IDIC, Y6, and PC₇₀BM Anna Leo <i>University of Salerno, Italy</i>
16:10	A Computational Study of Organic Molecular Crystals for Photocatalytic Water Splitting James Green <i>Imperial College London, UK</i>
16.15	Discussion
17:30	Lightning presentations (by invitation of the Scientific Committee)
18:00	Poster session and wine reception
19:30	Close

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Thursday 2 July 2026 (all timings are BST)

	Session 2: Advances in experimental design and synthesis of optoelectronic materials (Session chair: Ryan Crisp)
09:00	Measuring the liquidus of the Ba-Zr-S system and implications for flux-assisted growth of BaZrS₃ Rafael Jaramillo <i>MIT, USA</i>
09:05	Interface Engineering: A Step Towards Device Integration of Chalcogenide Perovskites Rakesh Agrawal <i>Purdue University, USA</i>
09:10	The Effect of the Sulfur Source on BaZrS₃ Low-Temperature Crystallization: H₂S vs. Elemental Sulfur Anat Itzhak <i>Technical University of Denmark, Denmark</i>
09:15	Composition Dependence of Electronic Defects in BaZrS₃ Thin Films Sulfurized from Oxide Precursors Adriana Röttger <i>Helmholtz-Zentrum Berlin, Germany</i>
09:20	Discussion
11:00	Refreshments
11:30	Unraveling the tunable transient optical response of colloidal 2D Mo_{1-x}W_xS₂ nanosheets. Jannika Lauth <i>Universität Tübingen, Germany</i>
11:35	Exploration of the (Sb, Bi)2(S, Se)3 system for photovoltaics and SWIR sensors Jessica de Wild <i>IMEC, Belgium</i>
11:40	Phase Regulation via Dual Additives for Pure-blue Emitting Quasi-2D Perovskite Light Emitting Diodes Byungha Shin <i>KAIST, South Korea</i>
11:45	Discussion
13:00	Lunch
	Session 3: Advanced characterization techniques of optoelectronic materials (Session chair: Jose Marquez)
14:00	THz spectroscopy and deviation from Drude model of LT-GaAs thin films with sub-picosecond charge-carrier lifetime Jasmin-Clara Buerger <i>University of Oxford, UK</i>
14:05	Atomic structure and structural disorder vs. device efficiency in Kesterite monograin solar cells Susan Schorr <i>Helmholtz-Zentrum Berlin for Materials and Energy, Germany</i>
14:10	Discussion
15:00	Refreshments
15:30	From Spacer Engineering to Defect Dominance: Contrasting A₂PbBr₄ and A₄AgBiBr₈ Layered Perovskites Igal Levine <i>The Hebrew University of Jerusalem, Israel</i>
15:35	High-efficiency hybrid halide perovskites: a complex material with a simple start in the crystallization process

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	Ana Palacios Saura <i>Helmholtz-Zentrum Berlin, Germany</i>
15:40	Decoupling Amine Evolution from Sulfur Delivery in High-Temperature Metal Sulfide Nanocrystal Synthesis Ryan W. Crisp <i>Friedrich-Alexander-Universität, Germany</i>
15:45	Discussion
17:00	Close of sessions
19:30	Conference dinner

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Friday 3 July 2026 (all timings are BST)

	Session 4: Accelerating materials design with data science (Session chairs: Andrea Crovetto and Lucy Whalley)
09:00	Exploring self-driving labs for optoelectronic materials Jonathan Staaf Scragg <i>Uppsala universitet, Sweden</i>
09:05	ML-guided screening of chalcogenide perovskites as solar energy materials Diego Alejandro Garzón Castellanos <i>INL- International Iberian Nanotechnology Laboratory, Portugal</i>
09:10	Discovering new photovoltaics using optimal transport theory Keith Butler <i>University College London, UK</i>
09:15	Discussion
10:30	Refreshments
11:00	Clever Materials: When Models Identify Good Materials for the Wrong Reasons Kevin Maik Jablonka <i>Jena Center for Soft Matter, Germany</i>
11:05	Digital infrastructure to support daily high-throughput experimental materials research Lena Angelika Mittmann <i>DTU, Denmark</i>
11:10	Discussion
12:00	Concluding remarks lecture (Session chair: Mirjana Dimtrievska) Andriy Zakutayev <i>National Renewable Energy Laboratory, USA</i>
12:30	Acknowledgements and presentation of poster prizes
12:45	Close of meeting and lunch

Please note that this is a draft programme and timings may change.