11th International Conference on
Hard X-ray Photoelectron Spectroscopy

HAXPES2026

13th – 17th April 2026
Worcester College, Oxford, UK

Conference Handbook

Hosted by diamond

At-a-glance programme

Monday 13th April

08:30	Registration
09:00	Welcome
09:10	Lightning Introductions
	Career Snapshots
09:25	Dr Fernando Garcia-Martinez
09:35	Dr Curran Kalha
09:45	Dr Elisabetta Arca Scienta Omicron
09:55	Dr Ad Ettema
10:15	Break
11:00	Panel discussion
12:00	Lunch
13:00	Harwell Campus visit
17:00	Registration
17:30	Welcome and Drinks Reception

Tuesday 14th April

8:30	Registration
09:00	Conference Opening Prof Gianluigi Botton
	Instrumentation and Method Development
09:10	Dr Sakura Pascarelli
09:55	Dr Tommaso Pincelli,
10:20	Russell Egdell
10:35	Coffee Break
11:00	Dr Kateryna Artyushkova
11:25	Olivier Renault
11:40	Wilson Quevedo
11:55	David Cant
12:10	Oliver Rehm
12:25	Lunch
	Application I - Electronic Structure and Emergent Phenomena
13:30	Dr Ashish Chainani
14:15	Dr Claudia Cancellieri
14:40	Alexander Gray
14:55	Coffee Break
15:30	Assist. Prof Yan Wang
15:55	Deepnarayan Biswas
16:10	L. Plucinski
16:25	Nick Barrett
16:40	Andreas Fuhrberg
16:55	Raphaël Salazarsen
17:10	Sponsor talk by Dr Ad Ettema, International Sales Manager, Scienta Omicron
17:30	Poster Session & Drinks
19:00	Speakers' Dinner

Wednesday 15th April

8:30	Registration
	Application I - Electronic Structure and Emergent Phenomena
09:00	Prof Tomohiko Saitoh
09:25	Shigenori Ueda
09:40	Akira Sekiyama
09:55	Eugenie Martinez
10:10	Goro Nozue
10:25	Coffee Break

10:55	Hongliang Zhang
11:10	Dirk Hauschild
	Theory and Modelling
11:25	Prof Frank de Groot
12:10	Shiyang (Ann) Lu
12:25	Lunch
14:15	Assoc Prof Atsushi Hariki
14:40	Simone Ritarossi
14:55	Prof Dr Ján Minár
15:20	Coffee Break
	Instrumentation and Method Development
15:50	Jessica McChesney
16:05	Fernando García Martinez
	Federico Motti
16:20	Okkyun Seo
16:35	Jean-Pascal Rueff
16:50	
17:05	Walking Tour of Oxford
19:00	Conference Dinner (Balliol College)

Thursday 16th April

8:30	Registration
	Application II - Energy Materials Catalysis
09:00	Dr Christoph Schlueter
09:45	Prof Louis Piper
10:10	Yanis Jugie
10:25	Rosalía Cid Barreno
10:40	Coffee Break
11:10	Dr Prajna Bhatt
11:35	Galo Paez Fajardo
11:50	Robert Weatherup
12:05	Rahul Mahavir Varma
12:20	Pilar Ferrer
12:35	Lunch & IAB meeting
13:30	Alessandro Mirabelli
13:45	Kevin Lovelock
14:00	Freddy Enrique Oropeza
14:15	Orlando Castellano
15:00	Blenheim Palace Tour

Friday 17th April

8:30	Registration
	Atomic and Molecular
09:00	Dr Tatiana Marchenko
09:25	Prof Philip Moriarty
09:50	Matjaž Žitnik
10:20	Dr Ralph Püttner
10:45	Coffee Break
	Application I - Electronic Structure and Emergent Phenomena
11:10	Niclas Tilgner
11:25	Joachim Wollschläger
11:40	Yoshiyuki Yamashita
12:10	Close
12:30	Lunch

Contents

Welcome

Welcome to HAXPES2026, and to the historic city of Oxford. It is a great pleasure to host you at Worcester College, whose beautiful gardens and collegiate setting provide an inspiring backdrop for scientific exchange and discussion.

The International Conference on Hard X-ray Photoelectron Spectroscopy (HAXPES) has become a key meeting point for our community, and we are delighted to welcome you to its 11th edition. Held every two years, the HAXPES conference brings together researchers from academia, national laboratories, and industry to share advances in instrumentation, methodology, theory, and a wide range of applications.

This year's programme features a rich mix of plenary and invited presentations from leading experts, alongside contributed talks and poster sessions that highlight the breadth and vitality of the field. Alongside core developments in HAXPES, we are particularly excited to highlight emerging directions and new opportunities in related areas, including advances at X-ray free-electron lasers and other next-generation light sources. By bringing these perspectives together, we hope to spark new ideas, connections, and collaborations across the community.

We are very grateful to all those who have contributed to making this conference possible. In particular, we thank the members of the local organising team and the international advisory board, our institutional partners, sponsors, and exhibitors for their invaluable support. We also acknowledge the many speakers and contributors whose work forms the heart of this meeting.

Finally, we would like to thank all of you, our delegates, for joining us in Oxford. Your participation, discussions, and exchange of ideas are what make the HAXPES conference such a vibrant and rewarding event. We hope you enjoy both the scientific programme and the opportunity to connect with colleagues old and new in this unique setting.

Professor Anna Regoutz, University of Oxford and **Dr Tien-Lin Lee,** Diamond Light Source

Conference Chairs

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General Information

Conference office

For all enquiries during HAXPES, please visit the reception desk in the foyer of the Sultan Nazrin Shah Centre, next to the lecture theatre. The desk will be manned during the hours below. If you require any further assistance during the conference, please email events@diamond.ac.uk or call +44 (0)7741385214.

Medical and emergency services

If you require emergency medical assistance, please call 999 from any phone. You should call the NHS 111 service if you need medical help fast, but it is not a 999 emergency. Calls to 999 and NHS 111 are free from landlines and mobile phones.

Smoking policy

Smoking is not permitted inside College buildings. We ask that you please use the designated smoking areas and use the receptacles provided for cigarette ends.

Name badges and security

All delegates will receive a name badge upon registration. This badge is the official pass and must be worn to obtain entry to all HAXPES 2026 sessions.

Catering

All lunches and refreshments will be served in the foyer.

Wi-Fi

Worcester College is part of *Eduroam*. Should you have an *Eduroam* account through your institution, you will be able to connect to the Wi-Fi. Alternatively, complimentary Wi-Fi is available throughout the College, via the University Cloud network

Founded in 1714, Worcester College has been a meeting place for over 300 years. The college offers a world-class venue for conferences and events, including the Sultan Nazrin Shah Centre which is hosting HAXPES 2026.

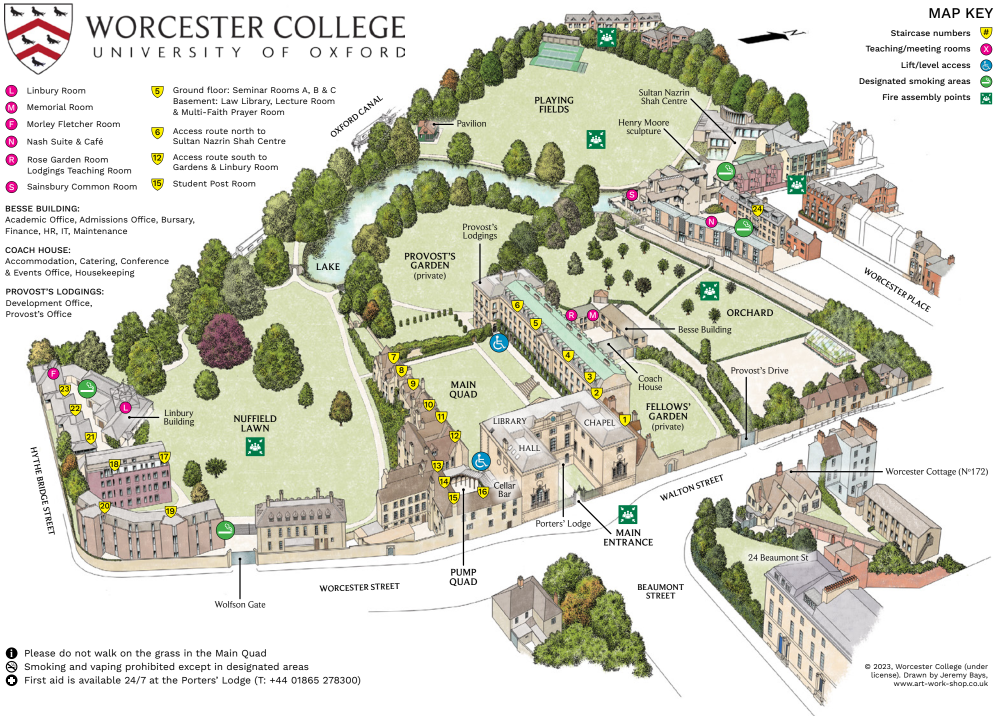
Worcester College is in central Oxford, just across from the main bus and coach station and a 10-minute walk from the railway station. It is close to the heart of the University of Oxford's iconic buildings, and to the main shopping areas of the city.

Please note that there are no car parking facilities available within the college. The use of public transport to and from Oxford is strongly recommended.

Address: Worcester College, Oxford,
OX1 2HB, United Kingdom

Travelling to and from Worcester College

If you are driving to Worcester College: The College is unable to offer parking on site. The nearest public car park is at the bottom of Worcester Street. This is accessed via Park End Street entrance and is fairly expensive. There are Four Park & Ride Bus Routes that provide buses to the City Centre approximately every 10 minutes; a charge is made for the bus ride and parking. Please visit www.oxfordshire.gov.uk/cms/public-site/park-and-ride for further details. Further short stay parking can be found on St Giles.



There is a small bicycle rack inside the college (also lots of bike racks round the corner at the Said Business School near the train station).

If you arrive by bus from another town: The bus station is located at Gloucester Green just off Worcester Street. Exit on to Worcester Street and walk towards Walton Street, the College is on your left. This will take approximately 5 minutes.

If you arrive by train at Oxford Station: Cross over the forecourt. Turn left out of the station and walk along Hythe Bridge Street then bear left on to Worcester Street until you reach the junction with Beaumont Street and Walton Street. It is approximately a 10-minute walk. There are several local buses and taxis available from the station if you prefer.

Taxis

The nearest taxi ranks are in Gloucester Green or at the train station. Taxis can also be booked in advance. Reliable taxi firms can be called on the following numbers: (+441865) 242424, 201201, 240000, 775577, and 770000.

Public transport

Oxford has an extensive network of local buses. The three main companies are Oxford Bus Company, Stagecoach and Thames Travel.

www.stagecoachbus.com
www.oxfordbus.co.uk

Social programme and facility tour

This information is only for those who have signed up for these activities in advance.

Harwell Campus tour

Monday 13 April 14:00-16:30

Meeting Location: Playhouse Theatre, Beaumont Street

Pick-up time: 13:00

Return trip: 16:30

A visit to Diamond Light Source's Structures and Surfaces Group beamlines and an overview of the Central Laser Facility (CLF).

Please remember to bring a valid, original government-issued photo ID (passport or driving licence). Photocopies or digital copies cannot be accepted, and access may be denied without the correct documentation. If you have any mobility requirements, please let the Diamond Events Team know in advance.

Oxford city tour

Wednesday 15 April 17:00-18:00

Meeting Location: Worcester College

Meeting time: 16:55

A Journey Through Oxford's History

Oxford has been at the centre of English history for over a thousand years, from being one of Alfred the Great's chosen cities, to the

invention of the Astra-Zeneca Covid vaccine. Traverse the historic streets and see the famous landmarks of the city and the University, while our expert guides share with you their knowledge of Oxford and its stories over the centuries. With many guides current students or alumni of the famed University, you can catch a glimpse into life here and now or be immersed in the lives of the people of the past and how they shaped Oxford, such as the Oxford Martyrs, King Charles I, and C.S. Lewis. Walk around the architectural monuments recognised around the world, such as the Radcliffe Camera, the Bodleian Library, and wander down the hidden passageways which lead to Oxford institutions such as the Turf Tavern, synonymous with US President Bill Clinton and Australian Prime Minister Bob Hawk. The guides offer a unique experience, adding their own flavour and expertise to each tour. This award-winning tour of Oxford offers an excellent opportunity to explore the city and see its famous "Dreaming Spires". The city centre of Oxford is relatively flat, and our easy paced tours can be tailored for most visitors. Some streets may be cobbled and caution and suitable footwear is recommended.

Blenheim Palace tour

Thursday 16 April 16:00-17:00 Private Guide Tour

Meeting Location: Playhouse Theatre, Beaumont Street, Oxford

Pick-up time: 15:00

Return trip: 17:30

Blenheim Palace is a country house in Woodstock, Oxfordshire, England. It is the seat of the Dukes of Marlborough. Originally called Blenheim Castle, it has been known as Blenheim Palace since the 19th century. One of England's largest houses, it was built between 1705 and 1722, and in 1987 it was designated a UNESCO World Heritage Site. The Palace and its parkland, often described as a "naturalistic Versailles," reflect the beginnings of the English Romantic movement and hold deep historical associations. The State Room tour offers guests an in-depth tour through lavishly decorated rooms such as the Great Hall, Saloon and Long Library. You'll see collections such as tapestries, antique furniture and paintings over 300 years old. The guide will also share stories about connection to the Duke of Marlborough past and present and the role in the birthplace of Winston Churchill.

Daily programme

Monday 13th April	
	EARLY CAREER MORNING
08:30	**Arrival & Registration**
09:00	**Welcome**
09:10	**Attendee Lightning Introductions** Quick intro round for everyone in attendance
	Career Snapshots (10 min each + 10 min buffer)
09:25	Dr Fernando Garcia-Martinez, Beamline Researcher at Beamline P22/Petra III (DESY)
09:35	Dr Curran Kalha
09:45	Dr Elisabetta Arca, Senior Lecturer and Future Leaders Fellow, Department of Physics, University of Liverpool
09:55	Dr Ad Ettema, International Sales Manager, Scienta Omicron
10:15	Coffee Break and Networking
11:00	**Panel discussion and live Q&A** Drs Garcia-Martinez, Kalha, Arca and Ettema **Chair:** Prof Anna Regoutz
12:00	Lunch
13:00	Harwell Campus Excursion (Diamond and CLF)
17:00	Arrival & Registration
17:30	Welcome by the Organisers and Drinks Reception

Tuesday 14th April

8:30	Arrival & Registration
09:00	Conference Opening Prof Gianluigi Botton, Chief Executive Officer, Diamond Light Source, UK
	Instrumentation and Method Development **Chair:** Prof Anna Regoutz, University of Oxford, UK
09:10	**Plenary Talk** – Dr Sakura Pascarelli, European XFEL, Germany X-ray Spectroscopy at the European X-ray Free Electron Laser
09:55	**Invited Talk** – Dr Tommaso Pincelli, Technical University Berlin and Fritz Haber Institute, Germany Towards femtosecond charge dynamics of active interfaces
10:20	**Contributed Talk** Robinson, Rutherford and Moseley: the birth of (hard) X-ray photoelectron spectroscopy Russell Egdell, University of Oxford, UK
10:35	Coffee Break
	Chair: Dr Tommaso Pincelli, Technical University Berlin and Fritz Haber Institute, Germany
11:00	**Invited Talk** – Dr Kateryna Artyushkova, PHI, USA Analysis of Interfaces by Soft and Hard X-ray Photoemission
	Contributed Talks
11:25	When HAXPES gets vertical: lab-scale analysis of GaN LED pixels sidewall after plasma etching Olivier Renault, CEA-Leti, Grenoble, France
11:40	Non-Destructive Depth Profiling by Variable Energy PARXPS (VE-PARXPS) Wilson Quevedo, SPECS Surface Nano Analysis GmbH, Berlin, Germany
11:55	HAXPES Analysis of Overlayers David Cant, National Physical Laboratory, Teddington, United Kingdom
12:10	Simulation-Guided GI-HAXPES: How to Maximize Signal and Depth Sensitivity in HAXPES Experiments Oliver Rehm, University of Konstanz, Konstanz, Germany

12:25	Lunch
	Application I - Electronic Structure and Emergent Phenomena **Chair:** Nick Barrett, CEA Saclay, Gif sur Yvette, France
13:30	**Plenary Talk** – Dr Ashish Chainani, Condensed Matter Physics Group, National Synchrotron Radiation Research Center, Taiwan Hard X-ray Photoelectron Spectroscopy of Metal-insulator, Magnetic and Charge-ordering Transitions in Strongly Correlated Materials
14:15	**Invited Talk** – Dr Claudia Cancellieri, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland Laboratory HAXPES/XPS for Depth-Resolved Chemical and Electronic Structures
14:40	**Contributed Talk** Probing the Origins of Emergent Superconductivity in Artificial High-Tc Superlattices with HAXPES Alexander Gray, Temple University, Philadelphia, United States
14:55	Coffee Break
	Chair: Prof Alex Gray, Temple University, Philadelphia, United States
15:30	**Invited Talk** – Assist. Prof Yan Wang, University of Cambridge, United Kingdom Semiconductor/dielectric interfaces in 2D semiconductor transistors

	Contributed Talks
15:55	Chirality in a Kagome Metal: a momentum microscope study Deepnarayan Biswas, Diamond Light Source, Didcot, United Kingdom
16:10	Single domain spectroscopic signatures of a magnetic Kagome metal L. Plucinski, Forschungszentrum Juelich GmbH, Juelich, Germany
16:25	Quantifying the oxygen vacancies and charge injection in ferroelectric hafnia-based devices Nick Barrett, CEA Saclay, Gif sur Yvette, France
16:40	Multimodal Photoelectron Spectroscopy of Ge-Based Hole Spin Qubit Heterostructures for Device Optimization Andreas Fuhrberg, Universität Konstanz, Konstanz, Germany
16:55	Probing the interface chemistry of a WSe_2/ferroelectric heterostructure at the microscopic scale Raphaël Salazar, Synchrotron Soleil, Gif-sur-Yvette, France and University of West Bohemia - NTC, Pilsen, Czechia
17:10	**Sponsor Talk – Scienta Omicron** Dr Ad Ettema, International Sales Manager, Scienta Omicron **Chair:** Prof Anna Regoutz, University of Oxford, UK
17:30	Poster Session & Drinks Reception
19:00	Speakers Dinner (St Edmund Hall)

Wednesday 15th April

8:30	Arrival & Registration
	Application I - Electronic Structure and Emergent Phenomena **Chair:** Dr Claudia Cancellieri, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland
09:00	**Invited Talk** – Prof Tomohiko Saitoh, Department of Applied Physics, Tokyo University of Science, Japan Electronic structure and oxygen-defect distribution of bulk single-crystalline In-Ga-Zn oxides revealed by hard x-ray photoemission spectroscopy
	Contributed Talks
09:25	Impact of spin-wave excitations on electronic states of half-metallic Co_2MnSi studied by temperature-dependent hard x-ray photoemission spectroscopy Shigenori Ueda, National Institute for Materials Science, Tsukuba, Japan
09:40	Pseudogap electronic structure and disorder simultaneously probed by HAXPES for a candidate thermoelectric quasicrystal Akira Sekiyama, Graduate School of Engineering Science, The University of Osaka, Toyonaka, Osaka, Japan and RIKEN SPring-8 Center, Sayo, Hyogo, Japan
09:55	Lab-scale HAXPES for critical buried interfaces in III-V heterostructures Eugenie Martinez, CEA-Leti, Grenoble, France
10:10	Soft and hard x-ray photoemission spectroscopy on a strongly correlated Cd-Ce quasicrystal approximant Goro Nozue, Julius-Maximilians-Universität Würzburg, Würzburg, Germany and The University of Osaka, Osaka, Japan
10:25	Coffee Break

	Chair: Prof Anna Regoutz, University of Oxford, UK
	Contributed Talks
10:55	The Electronic Structure of n-type β-Ga_2O_3 Epitaxial Thin Films Studied by HAXPES and ab initio calculations Hongliang Zhang, Xiamen University, Xiamen, China
11:10	Hard and Soft X-Ray Photoelectron Spectroscopy for a Depth-Resolved Look at Defect States in Ga_2O_3 Transparent Conductive Oxides Dirk Hauschild, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany and University of Nevada, Las Vegas (UNLV), Las Vegas, United States
	Theory and Modelling **Chair:** Dr Ashish Chainani, Condensed Matter Physics Group, National Synchrotron Radiation Research Center, Taiwan
11:25	**Plenary Talk** – Prof Frank de Groot, Debye Institute for Nanomaterials Science, Utrecht University, Netherlands The interpretation of core level XPS spectral shapes
	Contributed Talk
12:10	From core to valence states: a comprehensive experimental and theoretical photoelectron spectroscopy study of proteinogenic amino acids Shiyang (Ann) Lu, University of Oxford, UK
12:25	Lunch
	Chair: Prof Frank de Groot, Debye Institute for Nanomaterials Science, Utrecht University, Netherlands
14:15	**Invited Talk** – Assoc Prof Atsushi Hariki, Department of Physics and Electronics, Osaka Metropolitan University, Japan X-ray-Photoemission-Spectroscopy-Constrained DFT+DMFT Modeling of Correlated Materials
	Contributed Talk
14:40	Anisotropic recoil effects in hard-x-ray graphene C 1s photoemission Simone Ritarossi, Dipartimento di Scienze, Università degli Studi di Roma Tre, Rome, Italy

14:55	**Invited Talk** - Prof Dr Ján Minár, New Technologies Research Center (NTC), University of West Bohemia, Pilsen, Czech Republic One-step Photoemission Model: Core Levels to Valence Bands in Quantum Materials
15:20	Coffee Break
	Instrumentation and Method Development **Chair:** Dr Tien-Lin Lee, Diamond Light Source, UK
	Contributed Talks
15:50	Soft X-rays, Hard Questions: Identifying Band Character in Quantum Materials with ARPES Jessica McChesney, Argonne National Laboratory, Lemont, United States
16:05	Towards multi-modal and operando: simultaneous photoemission and structural measurements of gas–solid catalysts near 1 bar at beamline P22 Fernando García Martinez, Deutsches Elektronen Synchrotron DESY, Hamburg, Germany
16:20	The APE-TX project: a new HAXPES beamline at the Elettra 2.0 synchrotron Federico Motti, Elettra Sincrotrone Trieste and CNR - Istituto Officina dei Materiali (IOM), Trieste, Italy
16:35	Multimodal measuring system for chamberless HAXPES and XRD at the BL46XU beamline of SPring-8 Okkyun Seo, JASRI, Sayo, Japan
16:50	HAXPES at 4th generation synchrotron Jean-Pascal Rueff, Synchrotron SOLEIL, St Aubin, France
17:05	Walking Tour of Oxford
19:00	Conference Dinner (Balliol College)

Thursday 16th April	
8:30	Arrival & Registration
	Application II - Energy Materials Catalysis **Chair:** Assoc Prof Atsushi Hariki, Department of Physics and Electronics, Osaka Metropolitan University, Japan
09:00	**Plenary Talk** – Dr Christoph Schlueter, Beamline P22, Deutsches Elektronen-Synchrotron (DESY), Germany P22 at PETRA III: A Versatile Platform for Advanced HAXPES Studies
09:45	**Invited Talk** – Prof Louis Piper, WMG, University of Warwick, United Kingdom Oxygen Redox in Batteries: The Hole Picture
	Contributed Talks
10:10	From Surface to Bulk: Chemical and Electronic Structure Evolution of Delithiated LiNi0.8Mn0.1Co0.1O$_2$ Electrodes - Insights Into pSEI Formation and Redox Mechanisms with Lab-Based Coupled Soft and Hard XPS Yanis Jugie, Univ. Grenoble Alpes, CEA-LITEN, Grenoble, France
10:25	Dynamic interphases in halide solid-state batteries revealed by operando XPS: open questions for HAXPES Rosalía Cid Barreno, CIC energiGUNE, Vitoria-Gasteiz, Spain
10:40	Coffee Break
	Chair: Dr Christoph Schlueter, Beamline P22, Deutsches Elektronen-Synchrotron (DESY), Germany
11:10	**Invited Talk** – Dr Prajna Bhatt, Istitutio Officina dei Materiali, Consiglio Nazionale delle Ricerche (CNR-IOM), Italy Lifetime effects and satellites in the photoelectron spectrum of platinum metal

	Contributed Talks
11:35	The Hidden Surface Transformation That Limits Ni-Rich Li-Ion Batteries Galo Paez Fajardo, University of Warwick, Coventry and The Faraday Institution, Didcot, United Kingdom
11:50	Investigating the Contributions of Solid Electrolyte Interphases to the Electrochemical Stability Window of Aqueous Electrolytes in Li-Ion Batteries Prof Robert Weatherup, Department of Materials, University of Oxford
12:05	Impact of PEAI Passivation on Buried Interfaces in PSCs Probed by Operando HAXPES Rahul Mahavir Varma, Condensed Matter Physics of Energy Materials, Division of X-ray Photon Science, Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden
12:20	Zinc depletion at the $ZnFe_2O_4$ (1 1 1) single crystal surface: X-ray spectroscopy (NEXAFS and XPS) experiments and computer simulations Pilar Ferrer, Diamond Light Source, Didcot, United Kingdom
12:35	Lunch & IAB meeting

	Chair: Prof Louis Piper, WMG, University of Warwick, United Kingdom
	Contributed Talks
13:30	Interfacial Chemistry Limits the Stability of Deep Blue Perovskite LEDs Revealed by Operando Characterization Alessandro Mirabelli, University of Cambridge, Cambridge, United Kingdom
13:45	Ligand Donor Number from Potassium X-ray Photoelectron Spectroscopy Kevin Lovelock, University of Bath, Bath, United Kingdom
14:00	Bismuth-Based Photoelectrodes Unveiled by HAXPES: Probing the Contribution of Bi 6s and Bi 6p to the valence band Freddy Enrique Oropeza, IMDEA Energy, Madrid, Spain
14:15	A depth resolved investigation of hydrogen uptake in carbon based nanostructures Orlando Castellano, Università Degli Studi Roma Tre and INFN Sezione di Roma Tre, Rome, Italy
15:00	Excursion – Blenheim Palace Bus leaves at 15:00 for the tour at 16:00.

Friday 17th April

8:30	Arrival & Registration
	Atomic and Molecular **Chair:** Prof Dr Ján Minár, New Technologies Research Center (NTC), University of West Bohemia, Pilsen, Czech Republic
09:00	**Invited Talk** – Dr Tatiana Marchenko, CNRS (French National Centre for Scientific Research), France Charge transfer in organic molecules probed by resonant Auger spectroscopy
09:25	**Invited Talk** – Prof Philip Moriarty, School of Physics & Astronomy, University of Nottingham, United Kingdom Timing the Escape of a Caged Electron

	Contributed Talks
09:50	Auger decay from doubly excited core-hole states with sub-natural resolution: the Ar K case Matjaž Žitnik, J. Stefan Institute, Ljubljana, Slovenia
10:05	**Invited Talk** – Dr Ralph Püttner, Fachbereich Physik, Freie Universität Berlin, Germany Electron spectroscopy of isolated and solvated atoms using hard X-ray synchrotron radiation
10:30	Coffee Break
	Application I - Electronic Structure and Emergent Phenomena **Chair:** Dr Tien-Lin Lee, Diamond Light Source, UK
	Contributed Talks
11:10	X-ray Standing Wave Imaging: Structure Determination of 2D Materials with Hard X-rays Niclas Tilgner, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany
11:25	Structure and Electronic Properties of Epitaxial Ultrathin Ni-Fe oxide Films on MgO(001) Joachim Wollschläger, University of Osnabrück, Osnabrück, Germany
11:40	Lab-scale HAXPES for critical buried interfaces in III-V heterostructures Eugenie Martinez, CEA-Leti, Grenoble, France
11:55	The origin of the Fermi level pinning for Hf-based gate stack structures studied by operando hard x-ray photoelectron spectroscopy Yoshiyuki YAMASHITA, National Institute for Materials Science, Tsukuba, Japan and Kyushu University, Fukuoka, Japan
12:10	Conference Closing
12:30	Lunch and Departure

Methods Tuesday, 14th April, 09:10 (PLENARY)

Dr Sakura Pascarelli
European XFEL, Germany

Sakura Pascarelli received a Laurea in Physics at the University La Sapienza (Rome, Italy) and a PhD degree in Physics at the University Joseph Fourier (Grenoble, France). She moved to INFN (Frascati, Italy) in 1990, then to ESRF (Grenoble, France) in 1993, where her main scientific activity focused on the investigation of matter at extreme conditions of pressure, temperature and magnetic field. There she took over several managerial roles and responsibilities (XAS beamlines ID24 and BM23, Head of the Electronic Structure and Magnetism Group then Head of the Matter at Extremes Group). In September 2019 she joined the European XFEL (Hamburg, Germany) as Scientific Director responsible for the development of the scientific program of the four hard X-ray instruments.

X-ray Spectroscopy at the European X-ray Free Electron Laser

Sakura Pascarelli
European XFEL, Schenefeld, Germany

X-ray Free Electron Laser are opening novel avenues in the investigation of fundamental processes in many areas of science, from physics to chemistry, biology, and materials science, because they allow investigation of matter at the time scales of electron and nuclear dynamics, with chemical selectivity and bulk sensitivity.

In this talk I will briefly introduce the European XFEL and show a few examples of recent science highlights. I will focus on the X-ray spectroscopy platforms that are operational at both soft and hard X-ray instruments and illustrate their capabilities in different areas of research.

Finally, I will describe the newly commissioned Time-Resolved X-ray Photoelectron Spectroscopy (TR-XPS) platform and show some of the first user data. The commissioning of the Angle-Resolved TR-XPS mode is planned for later this year, and we hope to open it as soon as possible to user operation.

Methods Tuesday, 14th April, 09:55 (INVITED)

Dr Tommaso Pincelli
Technical University Berlin and Fritz Haber Institute, Germany

Tommaso Pincelli is a tenure-track research scientist at Technische Universität Berlin, where he leads the trARPES team in the Ultrafast Nanoscience group. His research focuses on ultrafast photoemission spectroscopy in 2D materials and heterostructures. His group investigates nonequilibrium electronic correlations in two-dimensional magnets and twisted heterostructures, with ongoing efforts in time-resolved hard X-ray photoelectron spectroscopy using European XFEL radiation. He has contributed to the design and operation of HHG-based photoemission beamlines and novel detection schemes multidimensional photoelectron spectroscopy. He received his PhD from the University of Milan and held postdoctoral positions at the Fritz Haber Institute and CNR-IOM.

Towards Femtosecond Charge Dynamics of Active Interfaces

Tommaso Pincelli[1,2], Alessandro De Vita[1,2], Gian Marco Pierantozzi[3], Alice Margherita Finardi[3], Michele Perlangeli[4,3], Riccardo Cucini[3], Martina Dell'Angela[3], Adnan Hammud[2], Patrick Grichtol[5], David Doblas Jimenez[5], Michael Heber[5], Manuel Izquierdo[5], Niclas Müller[6], Trideep Kawde[6], Pavel Trofimov[6], Hélène Seiler[6], Laurenz Rettig[2,7], Martin Wolf[2], Ralph Ernstorfer[1], Fausto Sirotti[4], Giancarlo Panaccione[3]

[1]Technische Universität Berlin, Berlin, Germany. [2]Fritz Haber Institut - MPG, Berlin, Germany. [3]Istituto Officina dei Materiali - CNR, Trieste, Italy. [4]Laboratoire de Physique de la Matière Condensée - École polytechnique, Paris, France. [5]European XFEL, Hamburg, Germany. [6]Freie Universität Berlin, Berlin, Germany. [7]Rheinland-Pfälzischen Technischen Universität, Kaiserslautern, Germany

As new strides are made toward faster and more compact devices, optoelectronics offers an appealing route to components that are smaller, more efficient, and faster. Combining femtosecond laser pulses with quantum materials enables the interplay between tailored light fields and unique material responses, opening the door not only to new functionalities but also to emerging physical phenomena. In hetero-structures, where the active element is an interface, optical excitation triggers complex charge and energy transfer processes that remain challenging to resolve.
To understand and potentially control these mechanisms, femtosecond core-level photoemission at high photon energies provides direct access to the electronic structure of buried interfaces under realistic operating

conditions—during optical excitation and several nanometers below the surface.
I will present our recent momentum microscopy studies at EuXFEL, where we directly probe ultrafast interfacial charge dynamics in two representative quantum material systems. In a layered semiconductor placed on a nanostructured plasmonic substrate, we observe rapid modifications of the electronic response following optical excitation, indicating efficient but complex charge transfer across the interface. In a wide-bandgap oxide (ZnO), we track the light-induced formation of a transient metallic state, revealing ultrafast carrier generation followed by slower redistribution and long-lived metastable behavior. These results highlight how interface structure and defects critically shape charge dynamics on femtosecond to nanosecond timescales.

Methods Tuesday, 14th April, 10:20

Robinson, Rutherford and Moseley: the Birth of (Hard) X-ray Photoelectron Spectroscopy

Russell Egdell
University of Oxford, Oxford, United Kingdom

Harold Roper Robinson was a leading pioneer of X-ray photoelectron spectroscopy (XPS) in the years between the two World Wars. He used hard X-rays from anodes including Cu, Mo and Ag to expel 'secondary cathode rays' from a range of target materials. The energies of the emitted electrons were analysed by deflection in a magnetic field, with detection on a photographic plate. Most of Robinson's results were presented as tables of binding energies, although he was also the first to publish a recognisable 'photoelectron spectrum'. He was also the first to report an XPS chemical shift – between the K-levels of Cr and $Cr(OH)_3$. This contribution will give an outline of Robinson's career. In particular it will explore how his early work in XPS was shaped by his interactions with Henry Moseley, when they both worked in the research group of Ernest Rutherford in Manchester in the years just before outbreak of the 1914-1918 World War. Moseley's famous experiments in X-ray emission spectroscopy started in Manchester and were completed in Oxford: they inspired Robinson to examine core levels with the technique he had first used to measure the energies of beta-rays. Moseley was killed in action in the pivotal battle of the Gallipoli campaign in 1915 and in his will he bequeathed his assets to the Royal Society. This led to establishment of a 'Moseley Studentship'. Robinson was the first recipient of this award, allowing him to resume his XPS experiments in Cambridge in the early 1920s.

Methods Tuesday, 14th April, 11:00 (INVITED)

Dr Kateryna Artyushkova
Physical Electronics, USA

Kateryna Artyushkova earned a Ph.D. in Analytical Chemistry from Kent State University and holds an M.Sc. and B.A. in chemical engineering from the National Technical University of Ukraine. After graduating, Kateryna held academic and research leadership roles at the University of New Mexico, including Research Associate Professor and Associate Director positions in multiple centers, as well as managing a surface analysis facility earlier in her UNM tenure. Kateryna joined Physical Electronics in September 2018 as a senior staff scientist working in Analytical Laboratory with a focus on the XPS product line. Since 2022, she is serving as a President of PHI. She has authored 270+ peer-reviewed papers. She is the North American Editor of Surface and Interface Analysis and an AVS Fellow.

Analysis of Interfaces by Soft and Hard X-ray Photoemission

Kateryna Artyushkova
Physical Electronics Inc, Chanhassen, United States

The benefits of having an X-ray of higher energy are apparent and have been discussed a lot in literature. Increasing the depth of analysis is an obvious advantage for analyzing buried interfaces. Analysis of reactive materials using combined soft and hard X-rays allows non-destructive resolution of in-depth compositional heterogeneities. Distinguishing surface enrichment of oxidation chemistries and their contribution to functions of materials such as catalysts and batteries is important application. One of the attractive advantages of using HAXPES is the ability to study buried interfaces and layers without worrying about ion beam damage during sputter depth profiles. In addition, combined XPS/HAXPES opens a way to accurately identify chemical phase using Auger parameter.

Together, I will use these examples to illustrate how combining soft and hard X-ray photoemission in a single laboratory instrument from Physical Electronics provides a powerful, non-destructive approach for chemical state analysis across the surface-to-bulk depth range, with broad applicability in energy materials, coatings, and surface science.

Methods Tuesday, 14th April, 11:25

When HAXPES gets Vertical: Lab-Scale Analysis of GaN LED Pixels Sidewall after Plasma Etching

Olivier Renault, Sandra Kozuch, Simon Ruel, David Vaufrey
CEA-Leti, Grenoble, France

The manufacture of pixels in gallium nitride (GaN)-based micro light-emitting diodes involves a plasma etching step, which results in material degradation at the pixel edges. This is particularly critical for small pixels and leads to a loss in the electro-optical efficiency of the GaN pixels. To address this issue, the development of etching processes generating lower material degradation is necessary (1). Improving etching makes essential proper to characterisation of the pixel sidewalls. To this end, we applied variable angle detection XPS/HAXPES on micron-scale patterns in the form of a set of arrays with different inter-pixel separation. The method exploits the shadowing created by neighbouring patterns (2) when the photoelectron take-off angle is matched with variable inter-pixel separation of two different pixel arrays. In HAXPES, two crucial advantages serve the goal of reliable analysis of the sidewall chemistry: firstly, the suppression of the overlap between Ga Auger and nitrogen core lines; secondly, the higher sensitivity to chlorine residues from the plasma enabled by the strong Cl 1*s* lines previously not accessible in XPS. As a side-result, the determination by XPS of the valence band maximum confirms the presence of plasma-induced defects in the GaN band gap, leading to non-radiative recombination of electron-hole pairs in the material thereby reducing its electro-optical efficiency at the pixel periphery.

(1) S. Kozuch et al., *J. Vac. Sci. Technol. A* 2026 (under review).
(2) R. Chanson et al., *J. Vac. Sci. Technol. B* 32, 011219 (2014).

Methods Tuesday, 14th April, 11:40

Non-Destructive Depth Profiling by Variable Energy PARXPS (VE-PARXPS)

Wilson Quevedo, Andreas Thissen
SPECS Surface Nano Analysis GmbH, Berlin, Germany

Chemical analysis of modern materials often requires characterization of both surface and bulk composition. EnviroMETROS LAB and FAB uses a monochromated, small-spot X-ray source with up to three photon energies and a wide-angle, angle-resolving electron analyzer to vary the kinetic energy and emission angle of the emitted photoelectrons. This enables highly sensitive, high-resolution measurements with direct, non-destructive depth profiling.

Variable-energy X-ray photoelectron spectroscopy (VE-XPS) employs tunable X-ray sources, such as synchrotrons or laboratory-based monochromators, to adjust the photon energy. By changing the photon energy, the kinetic energy of the emitted photoelectrons and thus the inelastic mean free path (IMFP) are controlled, allowing the analysis of surface, subsurface, and bulk regions with different sensitivities to selected core levels.

In parallel angle-resolved XPS (PARXPS), photoelectrons at different emission angles are collected simultaneously using the wide-angle analyzer AEOLOS 150 AD-CMOS. This parallel acquisition of spectra from multiple angles improves efficiency and precision for probing depth and electronic structure and allows the generation of concentration depth profiles.

Combining VE-XPS and PARXPS provides control over information depth and angular resolution, which is crucial for multilayer stacks and semiconductor structures. It enables clear discrimination between surface, interface, and bulk states, minimizes misinterpretation due to charging or deeper-layer contributions, and yields a much richer data set for precise and comprehensive characterization of material surfaces and interfaces.

Taken together, VE-XPS and PAR-XPS generate a much richer dataset, providing a better understanding.

Methods Tuesday, 14th April, 11:55

HAXPES Analysis of Overlayers

David Cant[1], Benjamen Reed[1], Jonathan Counsell[2], Anna Matiushkina[3], Robin Schuermann[4], Joerg Radnik[3], Ute Resch-Genger[3], Alexander Shard[1]

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The use of photoemission spectroscopy for analysis of layered systems is a well-established, reliable, and precise technique. The measurement of silicon oxide layers on silicon was one of the first standards developed under ISO for photoemission spectroscopies[1], and BIPM key comparisons have demonstrated that XPS is the most accurate technique for measurement of planar overlayers on the <10 nm scale[2]. Likewise, studies have shown the strength of XPS measurement of coatings on a variety of structures, including micro/nanoparticulate materials[3].

HAXPES instrumentation, with its greater information depths and broader energy range, improves this capability by allowing measurement of thicker overlayers, reducing sensitivity to coating inhomogeneity and, in tandem with traditional XPS, provides additional information, improving measurement accuracy. The challenge of how to combine information from different X-ray energies requires attention.

Here we outline methods to combine information and demonstrate the improvements provided by HAXPES when measuring coating thicknesses for samples with heterogeneous coatings, as well as for dealing with damaged overlayers e.g., as produced during ion beam sputtering. Examples of coating thickness measurement using both XPS and HAXPES for silica-coated iron particles and lanthanide-based up-conversion particles are shown and compared. Additionally, we show a method by which both techniques can be combined to obtain more accurate results than can be achieved by either alone. These methods and the advantages of HAXPES for measurements of coatings and overlayers are discussed in the context of the development of future standards for HAXPES under ISO.

1.ISO 14701
2.doi:10.1002/sia.1909
3.doi:10.1021/acs.jpcc.6b06713.

Methods **Tuesday, 14th April, 12:10**

Simulation-Guided GI-HAXPES: How to Maximize Signal and Depth Sensitivity in HAXPES Experiments

Oliver Rehm[1], Endirt Kusari[1], David Capalbo[1], Andreas Fuhrberg[1], Andrei Gloskovskii[2], Christoph Schlueter[2], Lutz Baumgarten[3], Martina Müller[1]

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[3]Forschungszentrum Jülich, Jülich, Germany

HAXPES is a powerful technique for probing the chemical and electronic structure of thin films, interfaces, and multilayers. However, access to synchrotron radiation is limited, and conventional HAXPES measurements are constrained by an "information cone" that integrates the signal over the full information depth (up to ~25 nm), thereby complicating the analysis and obscuring depth-specific features in layered devices.

To overcome this limitation, we present a simulation-guided approach for grazing-incidence HAXPES (GI-HAXPES). At incidence angles between 0.3° and 2°, X-ray refraction and total reflection generate pronounced angle-dependent interference, shifting the maximum weighted photoelectron yield to well-defined depths within the sample. The simulations predict these conditions a priori, enabling targeted surface-, interface-, or bulk-sensitive measurements. In combination with the angle-dependent photoelectron intensity (rocking curve), this approach provides access to layer thickness and depth-resolved chemical information. The confinement of the X-ray field within the upper few tens of nanometers enhances the photoelectron signal by up to two orders of magnitude.

In contrast to the depth averaging inherent to conventional HAXPES, simulation-guided GI-HAXPES allows continuous tuning of the probed depth by varying the incidence angle. This increases the information content and reduces ambiguity by separating overlapping contributions from different depth regions, while the enhanced intensity enables faster data acquisition with improved depth sensitivity. The methodology is demonstrated for a ferroelectric Pt/AlScN/Pt capacitor and will particularly benefit from next-generation synchrotron sources such as PETRA IV, where higher coherence and improved beam collinearity will further optimize the depth selectivity.

Application I Electronic Structure Tuesday, 14th April, 13:30 (PLENARY)

Dr Ashish Chainani
Condensed Matter Physics Group, National Synchrotron Radiation Research Center, Taiwan

Ashish Chainani obtained his B.Sc. (1985) and M.Sc. (1987) degrees from University of Mumbai, India, and his Ph.D. (1993) degree from the Indian Institute of Science, India. He did his post-doctoral studies at Tohoku University, Japan. He then joined Institute for Plasma Research, India, to work on plasma-based synthesis of materials for applied research. From 2003 to 2016, he worked as a Senior Research Scientist at RIKEN SPring-8 Center, Japan. Since 2016, he is working as a Scientist at the National Synchrotron Radiation Research Center, Taiwan. His research is focussed on using synchrotron-based spectroscopies for studying the electronic structure of materials which exhibit metal-insulator transitions, magnetic transitions, superconductivity, charge density waves and the Kondo effect.

Hard X-ray Photoelectron Spectroscopy of Metal-Insulator, Magnetic and Charge-Ordering Transitions in Strongly Correlated Materials

Ashish Chainani
National Synchrotron Radiation Research Center, Hsinchu, Taiwan

Hard X-ray Photoelectron Spectroscopy (HAXPES) has played a very important role in the last ~25 years, after its renaissance as a bulk-sensitive probe of the electronic structure of materials using third generation synchrotrons. HAXPES is now established as a reliable probe for studying basic and applied aspects of a wide range of materials spanning from semiconductors in device geometry to strongly correlated d- and f-electron materials exhibiting doping-dependent, temperature-dependent or thickness-dependent phase transitions (1,2). In this talk, we will focus on a few important cases which reflect the achievements, the diversity of materials and types of phase transitions for which HAXPES provided crucial inputs in understanding their properties: metal-insulator transitions in Mott-Hubbard and Charge-transfer materials (such as vanadates and cuprates), ferro- and ferrimagnetic transitions in rare-earth intermetallics and doped oxides, as well as charge-ordering transitions and Kondo effect in correlated systems. These results indicate that HAXPES provides unique and intrinsic aspects of the electronic structure while complementing other spectroscopies. HAXPES has a bright future in basic and applied sciences as a valuable tool for understanding the electronic structure of solids and its relation with their physical and chemical properties.

(1) *Hard X-ray Photoelectron Spectroscopy (HAXPES)*, edited by J. C. Woicik (Springer International Publishing, Switzerland, 2016), Vol. 59
(2) C. Kalha et al., Hard X-ray Photoelectron Spectroscopy: a snapshot of the state-of-the-art in 2020, Journal of Physics: Condensed Matter 33, 233001 (2021).

Application I Electronic Structure Tuesday, 14th April, 14:15 (INVITED)

Dr Claudia Cancellieri
Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Dr. Claudia Cancellieri is a group leader at Empa in the Laboratory for Joining Technologies and Corrosion. She received her PhD in Physics in 2008 from EPFL, specializing in pulsed laser deposition of cuprate and oxide thin films under strain. Following postdoctoral research at the University of Geneva and the Swiss Light Source at PSI, where she used advanced diffraction and spectroscopy techniques to study buried complex oxide interfaces, her research now focuses on the application of hard X-ray photoelectron spectroscopy (HAXPES) to investigate interfaces, chemical stability, and electronic properties of functional materials, including multilayers and thin amorphous oxides on metals.

Laboratory HAXPES/XPS for Depth-Resolved Chemical and Electronic Structures

Claudia Cancellieri
Empa, Swiss Federal Laboratories for Materials Science, Laboratory for Joining Technologies and Corrosion, Dübendorf, Switzerland

Hard X-ray photoelectron spectroscopy (HAXPES) extends conventional XPS by providing increased probing depth and access to Auger-parameter (AP)-based chemical state analysis. By combining XPS and HAXPES, core-level photoelectron and Auger lines can be depth-matched, enabling near-constant-depth chemical state analysis. In this contribution, several case studies demonstrate how AP shifts provide a highly sensitive probe of local chemical and electronic structure in diverse material systems. In metallic nanomultilayers, AP shifts sensitively reflect nondestructively electronic charge transfer and chemical intermixing at buried interfaces. For oxides, combined cation–anion chemical state analysis was performed on Ti- and Al-based oxide thin films prepared by different methods. Depth-resolved AP values were compared with bulk crystalline reference phases, revealing variations associated with differences in electronic polarizability between oxide polymorphs, changes in local coordination environments, and hydrogen incorporation in the oxides. In amorphous ALD-grown Al_2O_3, measured AP shifts as a function of film density and hydrogen content were successfully reproduced by atomistic simulations using machine-learning interatomic potentials, enabling identification of hydrogen-induced changes in the distribution of 4-, 5-, and 6-fold coordinated Al sites. Recently, an integrated electrochemical–UHV approach combined with XPS/HAXPES has been implemented to investigate the interaction of atomic hydrogen with passive oxides on steel. Finally, lab-based XPS/HAXPES has been applied to $Li_7La_3Zr_2O_{12}$ solid electrolytes, establishing reference data for identifying surface contamination and reaction layers. Extensions toward operando HAXPES provide new insight into interfacial dynamics during electrochemical cycling and their impact on battery performance.

Application I Electronic Structure **Tuesday, 14th April, 14:40**

Probing the Origins of Emergent Superconductivity in Artificial High-T_c Superlattices with HAXPES

Alexander Gray[1], Tien-Lin Lee[2], Gaetano Campi[3], Antonio Bianconi[4]

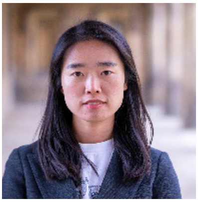
[1]Temple University, Philadelphia, United States. [2]Diamond Light Source Ltd., Didcot, United Kingdom. [3]IC-CNR, Rome, Italy. [4]RICMASS, Rome, Italy

A growing body of work has shown that oxide heterostructures can host interfacial superconductivity, highlighting the interface as a fertile platform for discovering new quantum states. A striking example is artificial high-T_C superlattices (AHTS) composed of overdoped $La_{1.55}Sr_{0.45}CuO_4$ and undoped La_2CuO_4, which exhibit interfacial superconductivity with an elevated critical temperature (1). Using hard X-ray photoelectron spectroscopy (HAXPES) and polarization-dependent soft X-ray absorption spectroscopy (XAS), we probe the occupied and unoccupied electronic structure across a series of superlattices with systematically varied geometries. We find spectroscopic evidence consistent with the formation of a superconducting dome in proximity to a topological Lifshitz transition, accompanied by Fermi-surface reconstruction and enhanced many-body screening at the resonance condition. Chemical-potential shifts extracted from La 3*d* core-level spectra pinpoint the Lifshitz regime. Complementary Cu L_3 and O *K*-edge XAS measurements reveal electronic signatures unique to the superconducting superlattices. Together, these results connect theoretical predictions with experimental observations and establish an electronic-structure basis for AHTS (2).

1. A. Valletta, A. Bianconi, A. Perali, G. Logvenov, and G. Campi, *Phys. Rev. B* **110**, 184510 (2024).
2. U. M. Jayathilake, S. Sheikh, T.-L. Lee, C. Klewe, G. Logvenov, G. Campi, A. Bianconi, and A. X. Gray, *in preparation* (2026).

Application I Electronic Structure **Tuesday, 14th April, 15:30 (INVITED)**

Assist. Prof Yan Wang
University of Cambridge, United Kingdom



Dr Yan Wang received her PhD from University of Cambridge in 2021 and become an independent PI at University of Cambridge in 2024. She is a research fellow at St John's College at Cambridge. Her research focuses on developing ultra-low power electronics based on two dimensional (2D) materials. She develops innovative methods to study atomic interfaces using imaging, spectroscopic, and electronic techniques, leveraging these approaches to investigate how the interfaces of 2D materials affect the overall device performance.

Semiconductor/Dielectric Interfaces in 2D Semiconductor Transistors

Yan WANG
University of Cambridge, Cambridge, United Kingdom

Atomically thin (or two-dimensional, 2D) transition metal dichalcogenide (TMD) semiconductors possess ideal attributes for meeting industry scaling targets for transistor channel technology. The realization of ultra-scaled field effect transistors (FETs) will require industry compatible gate dielectrics with very low equivalent oxide thickness (EOT) values (1). Dielectric substrates such as SiO_2, Al_2O_3 and HfO_2 unintentionally dope 2D TMDs and create interfacial defect states that lead to non-ideal FET characteristics – such as variable threshold voltage. Here we show that zirconium oxide (ZrO_2) forms an ultra-clean and inert interface with MoS_2 (2). Our detailed soft and hard X-ray photoelectron spectroscopy (XPS) analysis reveals that SiO_2 and HfO_2 substrates introduce significant doping of MoS_2 while ZrO_2 exhibits no measurable interactions with MoS_2. Because of the ultra-clean MoS_2/ZrO_2 dielectric interface, MoS_2FETs using ZrO_2 as dielectric show extremely stable and positive threshold voltage, low subthreshold swing, and high ON currents. Furthermore, we demonstrate that the ultra-clean interface between ZrO_2 and monolayer MoS_2 enables effective modulation of the threshold voltage in top gate FETs by gate metal work function engineering (3).

(1) Nature Electronics 7, 638–645 (2024)
(2) Nature Electronics 8, 906–912 (2025)
(3) arXiv:2512.20069

SPEAKERS

Application I Electronic Structure **Tuesday, 14th April, 15:55**

Soft X-ray Momentum Microscopy at the I09 beamline, Diamond Light Source, UK

Deepnarayan Biswas[1], Jieyi Liu[1], Olena Tkach[2], Olena Fedchenko[2], Hans-Joachim Elmers[2], Ralph Claessen[3], Gerd Schönhense[2], Tien-Lin Lee[1]

[1]Diamond Light Source, Didcot, United Kingdom. [2]Johannes Gutenberg-Universität, Mainz, Germany. [3]University of Würzburg, Würzburg, Germany

The K-branch of the I09 beamline at Diamond Light Source (DLS) is equipped with a state-of-the-art momentum microscope (MM) for investigation of electronic and structural properties of surfaces, buried interfaces and bulk crystals employing angle-resolved photoelectron spectroscopy (ARPES) and photoelectron diffraction (PED). The beamline delivers photons from 105 eV to 2 keV with variable polarisations, enabling probing of dichroic properties. Additionally, the availability of a photoelectron emission microscopy (PEEM) mode allows real-space imaging and spatially resolved k-space mapping (micro-ARPES). A hybrid mode that combines a hemispherical analyser (HSA) with time-of-flight electron detection enables ARPES measurements that are over an order of magnitude more efficient than conventional HSA-ARPES setups (1). Recent upgrades to the MM include a zero-field mode that suppresses electrical discharge during measurements of rough or cleaved samples (2).

Two scientific studies will be presented to demonstrate the unique capabilities of this instrument. In the kagome metal CsV_3Sb_5, we observed pronounced magnetic circular dichroism (MCD) in ARPES spectra, revealing a chiral electronic structure in the charge density wave (CDW) phase. Nb doping enhances the MCD signal while weakening the CDW order (3). Secondly, PED studies of Si (111) and Ge (111) at low kinetic energies reveal strong subshell-dependence of the diffraction patterns, underscoring the role of initial-state orbital structures in PED.

(1) Schmitt, M. et al. Ultramicroscopy **276**, 114169 (2025).
(2) Tkach, O. & Schönhense. Ultramicroscopy **276**, 114167 (2025).
(3) Elmers, H. J. et al. PRL **134**, 096401 (2025). Elmers, H. J. et al. PRB **112**, 245109 (2025).

Single Domain Spectroscopic Signatures of a Magnetic Kagome Metal

L. Plucinski[1], G. Bihlmayer[1], Y. Mokrousov[1], Yishui Zhou[1], Yixi Su[1], A. Bostwick[2], C. Jozwiak[2], J. Denlinger[2], E. Rotenberg[2], D. Usachov[3], C. M. Schneider[1]

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Spin- and orbital-resolved access to the electronic bands is necessary to establish key properties of quantum materials such as the quantum-geometric tensor. Despite the recent revival of interest in magnetic Kagome compounds, no spectroscopic access to their magnetic properties has been available so far due to small domain sizes and the lack of appropriate techniques. Furthermore, their real-space magnetic texture is often complex and temperature-dependent.

We investigate the magnetic Kagome metal $DyMn_6Sn_6$ using high-resolution micro-focused circular-dichroic angle-resolved photoemission (μ-CD-ARPES) to probe its magnetic and electronic properties. By tuning the kinetic energy to various features of the Dy *4f* multiplet, we resolve magnetic domains in samples cryo-cooled down to 20 K. Smaller, but clear, signatures are also detected in the Mn *3p* levels. The behavior of both Dy *4f* and Mn *3p* features is in remarkable agreement with our modeling based on the Hartree–Fock method, revealing ferrimagnetic alignment of Dy and Mn local moments and further strengthening our interpretation.

Adjusting the energy to the Mn *3d*-dominated valence bands reveals signatures that we relate to the orbital magnetization through comparison with *ab initio* electronic structure calculations. Our study establishes spectroscopic access to a single magnetic domain in a Kagome metal and demonstrates μ-CD-ARPES as a direct probe of magnetic domain properties, opening the way for spatially resolved studies of complex magnetic phases in quantum materials.

Reference: arXiv:2507.12085 (2025); accepted for publication in *Nature Communications.*

Application I Electronic Structure **Tuesday, 14th April, 16:25**

Quantifying the Oxygen Vacancies and Charge Injection in Ferroelectric Hafnia-Based Devices

Nick Barrett

CEA Saclay, Gif sur Yvette, France

Ferroelectricity in hafnia-based materials has opened the way to integration in non-volatile memory and logic, fully compatible with current silicon technologies. In particular, $Hf_xZr_{1-x}O_2$, has attracted much attention thanks to the low recrystallization temperature and wide range of phase stability.

Several flavours of ferroelectric hafnia-based devices, notably ferroelectric random-access memories (FeRAMs) and ferroelectric field effect transistors (FeFETs), suitable for back and front end of the line integrations, respectively. Amongst all emerging non-volatile memory technologies, ferroelectric hafnia offers by far the lowest power rating, in addition to being extremely low cost and suitable for aggressive 3D scaling.

The key performance parameters are the remanent polarization, the imprint or shift of the hysteresis loop along the voltage axis, the endurance in terms of operational cycles and retention. In this respect charged defects, specifically oxygen vacancies, and charge injection play a crucial role. Characterizing accurately the oxygen vacancy distribution in these sub-10 nm films, and their evolution with field cycling simulating operational use is therefore critical to industry.

We have used HAXPES to characterize a wide range of customized HZO based devices, both capacitor and transistor stacks, with a view to implementation as FeRAMs and FeFETs.

The effect of processing conditions, interface chemical engineering and field cycling on the oxygen vacancy concentration profiles has been quantified building a coherent picture of the defect chemistry in these stacks.

This work has received funding from the EU project n° 780302 3eFerro and 101135656 Ferro4EdgeAI, the ANR-DFG project D3PO and France 2030 project ANR-22-PEXD-0018.

Application I Electronic Structure **Tuesday, 14th April, 16:40**

Multimodal Photoelectron Spectroscopy of Ge-Based Hole Spin Qubit Heterostructures for Device Optimization

Andreas Fuhrberg[1], Maximilian Oezkent[2], Kevin-P. Gradwohl[2], Sergii Chernov[3], Volkmar Koller[3], Christoph Schlueter[3], Hans-Joachim Elmers[4], Martina Müller[1]

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Semiconductor spin qubits are a promising platform for quantum information processing. Although silicon-based electron spin qubits have been extensively studied, germanium-based hole spin qubits have emerged as an attractive alternative due to their favourable material and spin–orbit properties. These qubits are commonly realized in strain-engineered heterostructures, particular in $Ge_{0.8}Si_{0.2}$ /Ge/$Ge_{0.8}Si_{0.2}$ quantum wells. At the interfaces hole confinement is governed by a strain-induced valence band offset (VBO), a key parameter for device design and performance.

A set of three synchrotron-based experiments is performed to systematically investigate the two interfaces of Ge-based hole spin qubit heterostructures, varying the thickness of the central Ge layer and the $Ge_{0.8}Si_{0.2}$ overlayer. Hard X-ray momentum microscopy (MM) at different photon energies allows to resolve the valence band along the momentum directions Γ- X and Γ- L, enabling the VBO at each interface to be determined directly and individually. The measured band structure exhibits Ge-like heavy-hole/light-hole bands, as well as the spin-orbit split off bands, with an interface-induced increase of the spin–orbit splitting by approximately 50 meV.

Furthermore, additional MM-based photoelectron diffraction experiments observe structural and lattice-related modifications, while hard X-ray photoelectron spectroscopy at different photon energies provides complementary chemical information regarding the respective interface composition.

Combined, this three-in-one photoelectron spectroscopy technique enables a comprehensive characterization of the key electronic, structural and chemical properties of Ge-hole spin qubits, providing direct input for device optimization.

Application I Electronic Structure **Tuesday, 14th April, 16:55**

Probing the Interface Chemistry of a WSe_2/Ferroelectric Heterostructure at the Microscopic Scale

Raphaël Salazar[1,2], Cléophanie Brochard[3,4], Sara Varotto[5], Saleem Ayaz Khan[2], Thomas Maroutian[3], Jan Minar[2], Julien Chaste[3], Fabrice Oehler[3], Abdelkarim Ouerghi[3], Stéphane Fusil[5], Manuel Bibes[5], José Avila[1], Pavel Dudin[1], Chiara Bigi[1], François Bertran[1], Patrick Le Fèvre[1,6]

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Mixed dimensions heterostructures have become a large field of research for potential applications of transition metal dichalcogenides. Among them, promising efforts in the realm of IR-VIS photodetection, memory and transistors based on transition metal dichalcogenides and ferroelectric materials heterostructures have emerged. Despite major advances in the optical and electrical characterization of increasingly complex devices, these interfaces remain poorly understood. In this work, we investigate chemical vapor deposition (CVD) grown monolayer WSe_2 flakes interfaced with thin-film opposite polarized multiferroic $BiFeO_3$(001) (BFO) using microfocused photoemission spectroscopy (µ-XPS) at a synchrotron facility. We obtain hyperspectral images of our heterostructures that we analyze combining traditional peak-fitting procedures and automated clusterization algorithms to extract statistically relevant trends and core-level cartography. We compare those results with piezoelectric force microscopy (PFM) and µ-photoluminescence (µPL) spectroscopy images. Using core level information at the interface and flake boundaries, we discover that the TMD monolayer exhibit different charge transfer patterns depending on the termination of the BFO beyond the rigid shift picture and get evidence of a deeper bonding between the BFO and the WSe_2.

Application I Electronic Structure **Wednesday, 15th April, 09:00 (INVITED)**

Prof Tomohiko Saitoh
Tokyo University of Science, Japan

Tomohiko Saitoh is a professor of the Department of Applied Physics, Tokyo University of Science in Japan. He earned his Ph.D. in condensed matter physics from the University of Tokyo in 1996. After a postdoctoral position at the University of Colorado at Boulder, he became a beamline scientist at the Photon Factory, and then moved to the current university. He received several honors/awards including an Outstanding Referee of APS in 2014. He has long been working on photoelectron spectroscopy and also first-principles band-structure calculations. His research interests are the electronic structure and magnetism of solid-state compounds, particularly strongly correlated systems and functional materials such as 3*d* transition-metal oxides or transparent conductive oxides.

Electronic Structure and Oxygen-Defect Distribution of Bulk Single-Crystalline In-Ga-Zn Oxides Revealed by Hard X-ray Photoemission Spectroscopy

Tomohiko Saitoh[1], Goro Shibata[2]

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Owing to high transparency and high electrical conductivity, transparent conductive oxides (TCOs) have potential applications in display devices and solar cells, for example (1), thereby making them indispensable materials in modern society. Among them, $InGaZnO_4$, known as IGZO, is already used for thin-film transistors (TFTs) of flat-panel displays. Nevertheless, a critical issue remains to be resolved for improving IGZO-based TFTs, the negative bias illumination stress instability, which has often been attributed to the additional density of states at the valence-band maximum (VBM), called "subgap states". However, its origin has been a long-standing controversy. An important reason for this is that large bulk single-crystalline IGZOs (sc-IGZOs) for macroscopic measurements were unavailable, leading most studies to focus on amorphous IGZO (a-IGZO).

Recently, Tanaka *et al.* achieved the world's first successful synthesis of mm-sized bulk sc-IGZOs (2). We performed hard x-ray photoemission spectroscopy experiments for both as-grown and oxygen-annealed samples of these sc-IGZOs (3). We found that the near-VBM subgap states were negligibly weaker than in a-IGZOs, demonstrating that the crystallinity mostly explains the near-VBM subgap states. Our detailed core-level analyses also found that oxygen vacancies are preferentially located around In atoms in as-grown crystals, which may be relevant to the anisotropic transport properties of sc-IGZO (2).

We will also present recent advances in our research on other homologous members.

Application I Electronic Structure **Wednesday, 15th April, 09:25**

Impact of Spin-Wave Excitations on Electronic States of Half-Metallic Co_2MnSi Studied by Temperature-Dependent Hard X-ray Photoemission Spectroscopy

Shigenori Ueda[1], Yuichi Fujita[1], Ivan Kurniawan[1], Yuya Sakuraba[1], Yoshio Miura[1,2]

[1]National Institute for Materials Science, Tsukuba, Japan. [2]Kyoto Institute of Technology, Kyoto, Japan

We have performed the valence band hard x-ray photoemission spectroscopy for a half-metallic Co_2MnSi (CMS) thin film capped by a thin AlO_x layer to clarify the impact of spin-wave excitations on the electronic states in the low temperature (LT) region (20-300 K), which is predicted by the theoretical calculations combined with the disordered local moment (DLM) method for bulk CMS (1). We found that even the LT region (< 0.4 times of the Curie temperature), the spin-wave excitations affect the bulk electronic states of CMS, which depend on temperatures. The changes of electronic states of bulk CMS qualitatively agree with those obtained by the DLM calculations through the simulation of the valence band HAXPES spectra with considering the matrix element effect, suggesting the importance of spin-wave excitations on the electronic states of bulk CMS at finite temperatures (2). By using X-ray total reflection, the enhancement of the spin-wave excitations near the interface of the AlO_x/CMS film was detected by magnetic circular dichroism in core-level HAXPES. We also found that the valence band HAXPES spectra of CMS near the interface differ from those of bulk CMS (2). These results suggest that the direct observation of electronic and magnetic states of the insulator/ferromagnet heterojunctions in non-destructive way is important to reveal the properties of magnetic materials at finite temperatures.

(1) K. Nawa et al., Phys. Rev. B 102, 054424 (2020).
(2) S. Ueda, Y. Fujita, I. Kurniawan, Y. Sakuraba, Y. Miura, Phys. Rev. B, accepted.

Application I Electronic Structure **Wednesday, 15th April, 09:40**

Pseudogap Electronic Structure and Disorder Simultaneously Probed by HAXPES for a Candidate Thermoelectric Quasicrystal

Akira Sekiyama[1,2], Nonoka U. Sakamoto[1,2], Goro Nozue[1,2], Hidenori Fujiwara[1,2], Akira Yasui[3], Yasumasa Takagi[3], Yuto Torii[1], Mai Sakaguchi[1,2], Takuya D. Nakamura[1,2], Kenshin Okazaki[1,2], Takayuki Kiss[1], Satoru Hamamoto[2], Masaki Oura[2], Kiyofumi Nitta[3], Souta Tanaka[4], Yutaka Iwasaki[5], Yasuhiro Niwa[4], Asuka Ishikawa[4], Takafumi D. Yamamoto[4], Ryuji Tamura[4]

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So-called pseudogap electronic structure in the vicinity of the Fermi level (E_F) has often been reported for Al-based quasicrystals (QCs) (1,2), which are expected as candidates of thermoelectric materials. However, such reports have been based solely on the valence-band photoemission spectral weight. Here we have verified the intrinsic element-dependent pseudogap electronic structure of an Al-Pd-Ru QC by both valence-band and core-level hard X-ray photoemission spectroscopy (HAXPES), and x-ray absorption (XAS) (3,4). The valence-band HAXPES spectral weights, the asymmetry of the core-level HAXPES lineshapes, the recoil effects we have found by hn-dependent HAXPES, and the absorption-edge photon energies compared with the core-level binding energies indicate a slight contribution of the Al sites to the electronic structure in the vicinity of E_F with less contributions from the Pd and Ru sites. The disorder effects (5) are found in the core-level HAXPES of the Al-Pd-Ru QC, of which the widths are much broader than those of the other reference crystalline solids with less disorder. The degree of peak broadening is comparable among the Al, Pd and Ru sites, which also implies the presence of the pseudogap in the vicinity of E_F.

(1) J. Nayak *et al.*, Phys. Rev. Lett. **109**, 216403 (2012).
(2) S. Sarkar *et al.*, Phys. Rev. B **103**, L241106 (2021).
(3) N. U. Sakamoto, A. Sekiyama *et al.*, submitted to Phys. Rev. Mater.; arXiv:2505.11156.
(4) N. U. Sakamoto, A. Sekiyama *et al.*, Mater. Trans. in press.
(5) G. Nozue, A. Sekiyama *et al.*, J. Phys. Soc. Jpn. **93**, 074703 (2024).

Application I Electronic Structure **Wednesday, 15th April, 09:55**

Pseudogap and Anderson Localization in Quasicrystals

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Quasicrystals with forbidden symmetry and remarkable physical properties such as high resistivity and low thermal conductivity have fascinated scientists since their discovery. The stability of quasicrystals has been ascribed to a mechanism that predicts the existence of a pseudogap in the electronic density of states (DOS) at the Fermi level (E_F) due to quasi-Brillouin zone and Fermi surface interaction. However, the stability of the decagonal (*d*) quasicrystals that exhibit two-dimensional quasiperiodicity is unresolved to date. Employing hard X-ray photoelectron spectroscopy (HAXPES) and density functional theory (DFT), we demonstrate the existence of the pseudogap in the bulk electronic structure of *d*-Al-Ni-Co, which is associated with Al-transition metal bonding (1). However, the pseudogap is shallower compared to icosahedral (*i*) quasicrystals (2), which explains the lower resistivity of *d*-Al-Ni-Co. Disorder in a quasiperiodic lattice complicates its electronic structure leading to Anderson localization, as observed in polygrain *i*-Al-Pd-Re (3). HAXPES measurements reveal enhanced DOS at E_F in polygrain *i*-Al-Pd-Re compared to its single-grain counterpart. In contrast, the conductivity of the former is an order of magnitude reduced, indicating that these electron states are localized. DFT calculations attribute these states to Re 5*d*-Pd 4*d* hybridization.

We acknowledge the valuable contributions of all co-authors of Refs. 1 and 3 to the work presented here.

(1) S. Sarkar *et al.*Physical Review B **111**, 165126 (2025).
(2) J. Nayak *et al.* Physical ReviewLetters **109**, 216403 (2012).
(3) S. Sarkar *et al.* Physical Review B (Lett.) **103**, L241106 (2021).

Application I Electronic Structure Wednesday, 15th April, 10:10

Soft and Hard X-ray Photoemission Spectroscopy on a Strongly Correlated Cd-Ce Quasicrystal Approximant

Goro Nozue[1,2], Hidenori Fujiwara[2,3], Satoru Hamamoto[3], Miwa Tsutsumi[2,3], Akane Ose[2,3], Takayuki Kiss[2], Atsushi Higashiya[3,4], Atsushi Yamasaki[3,5], Yuina Kanai-Nakata[3,6], Shin Imada[3,6], Masaki Oura[3], Kenji Tamasaku[3], Makina Yabashi[3], Tetsuya Ishikawa[3], Shintaro Suzuki[7], Farid Labib[8], Ryuji Tamura[8], Akira Sekiyama[2,3]

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Rare-earth-based quasicrystals and their approximants show fascinating quantum states. Cd_6R (R: rare-earth element) 1/1 approximants have been recognized as prototypical systems for these alloys. Among them, Cd_6Ce exhibits a magnetic transition around 0.5 K (1). However, the magnetic ground state of Cd_6Ce has not been clarified. To address this issue, it is essential to reveal the hybridization effects between the localized 4*f* orbitals and the itinerant valence bands (c-*f* hybridization). In this study, we have performed the Ce 3*d*-4*f* resonant photoemission spectroscopy (RPES) and the hard X-ray photoemission spectroscopy (HAXPES) to investigate the c-*f* hybridization effects in Cd_6Ce (2,3).

In the on-resonance valence-band spectra, the spectral weight of the $4f^1_{5/2}$ final state is suppressed compared with that of the $4f^1_{7/2}$ final state, indicating that the c-*f* hybridization strength is weak at the Fermi level (E_F) in Cd_6Ce. Based on the linearly polarized HAXPES results, we have carried out the non-crossing approximation calculation within the framework of the single-impurity Anderson model. The simulated 4*f* spectrum well reproduces the on-resonance spectrum. In addition, it is found that the c-*f* hybridization strength well below E_F is much stronger than that at E_F, which differs from the c-*f* hybridization effect in the intermetallic Ce-based compounds. This anomalous hybridization effect is likely responsible for the unresolved magnetic ground state in Cd_6Ce.

(1) T. Shiino *et al.*, Phys. Rev. B **112**, 064418 (2025).
(2) G. Nozue *et al.*, J. Phys. Soc. Jpn. **93**, 074703 (2024).
(3) G. Nozue *et al.*, arXiv:2510.24277; submitted to Phys. Rev. B.

Application I Electronic Structure **Wednesday, 15th April, 10:55**

The Electronic Structure of n-type β-Ga_2O_3 Epitaxial Thin Films Studied by HAXPES and *ab initio* Calculations

Hongliang Zhang[1], Joe Willis[2], David Scanlon[3], Tien-Lin Lee[4], Duanyang Chen[5], Hongji Qi[5,6]

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Gallium oxide is emerging as a promising wide bandgap semiconductor for high-power electronics and solar-blind ultraviolet photodetector, due to its ulra-wide bandgap of 4.9 eV, high breakdown electric field of 8 MV/cm and availability of large size bulk crystal. The electronic structure and defect states of Ga_2O_3 thin films are crucial for device optimization. In this talk, we will report our recent studies on the electronic structures of Si and Sn doped n-type Ga_2O_3 epitaxial thin films with using a combination of HAXPES and density functional theory. The electronic states derived from Ga 4*s* character are selectively enhanced by HAXPES. Our work reveals that Si is a superior dopant over Ge and Sn, because Si 3*s* forms a resonant donor state above the conduction band minimum, leaving the host conduction band mostly unperturbed and a high mobility is maintained though the doping level is high. A comparison of the valence band spectra of Sn-doped Ga_2O_3 films with Si-doped samples suggests that Sn doping has different effects on the electronic structure than Si doping. An in-gap electronic state is observed for Sn-doped Ga_2O_3, which is attributed to self-compensating Sn^{2+} related defects. Furthermore, a larger band-gap renormalization is found in Sn-doped samples, because the Sn 5*s* dopant orbital mixes strongly with the host Ga 4*s* derived conduction band. Finally, a comparison of the valence band and core-level spectra excited with soft and hard X-rays allows us to identify an upward band bending at the surface region of Sn-doped Ga_2O_3 films.

Application I Electronic Structure **Wednesday, 15th April, 11:10**

Hard and Soft X-Ray Photoelectron Spectroscopy for a Depth-Resolved Look at Defect States in Ga_2O_3 Transparent Conductive Oxides

Dirk Hauschild[1,2], Elizaveta Pyatenko[1,3], Constantin Wansorra[1,2], Ralph Steininger[1], John Vinson[4], Wolfram Witte[5], Dimitrios Hariskos[5], Michael Powalla[5], Clemens Heske[1,2], Lothar Weinhardt[1,2]

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Transparent conductive oxides (TCOs) play a key role in a large variety of opto-electronic applications. In these materials, defect states are critical for the electronic properties and the device performance. The n-type conductivity of many TCOs is commonly attributed to oxygen vacancies. Other (unwanted) defects, in particular at interfaces, can also enhance charge-carrier recombination, which, diminishes the device performance. A detailed understanding of the electronic structure, especially of defect states and their impact on the band edges is therefore crucial.

In this contribution, we employ soft and hard X-ray photoelectron spectroscopy with excitation photon energies ranging from 0.1 to 6.3 keV, using the uniquely wide energy range of the X-SPEC beamline at the KIT Light Source. This allows for a systematic, depth-resolved probe of the electronic structure. We investigate a sputtered Ga_2O_3 TCO thin film, as used in Cu(In,Ga)Se_2 thin-film solar cells, and compare it with a cleaved β-Ga_2O_3 single-crystal surface, before and after an Ar^+-ion treatment. The experimental data is complemented by density functional theory (DFT)-based spectra calculations.

We find spectral intensity above the valence band maximum, which varies as a function of probing depth and can be attributed to defect-related states. We also discuss the importance of DFT-based spectra calculations to verify the linear extrapolations for the determination of valence band extrema. Our results provide direct and depth-resolved insights into the impact of defect states on the electronic structure of TCOs and give input for further optimization for the charge-carrier transport across interfaces.

Theory Wednesday, 15th April, 11:35 (PLENARY)

Prof Frank de Groot
Debye Institute for Nanomaterials Science, Utrecht University, Netherlands

Frank de Groot is professor of X-ray Spectroscopy in the Debye Institute of Nanomaterials Science at Utrecht University. His work reflects a concern with both the theoretical and the experimental aspects of X-ray spectroscopy, including both fundamental studies and applications. His current interest is in the use of X-ray spectroscopies for the study of the electronic and magnetic structure of condensed matter, in particular for transition metal oxides, nanoparticles and heterogeneous catalysts under working conditions.

The Interpretation of Core Level XPS Spectral Shapes

Frank de Groot
Utrecht University, Utrecht, Netherlands

The interpretation of core level XPS spectral shapes will be reviewed using the two-state cluster model as starting point to explain (at least conceptually) all XPS spectral shapes. The general characteristics of the two-state cluster model will be explained and using a series of examples the different interactions and phenomena will be highlighted. Respectively rare earths (4*f*), actinides (5*f*), transition metals (3*d*, 4*d* and 5*d*) and main group elements will be discussed. The crucial parameter in the two-state cluster model is the core hole potential Q. Actually important is not the core hole potential itself, but the difference in electronic state shifts due to the core hole potential; For example in a transition metal oxide the 3*d* states will shift more due to the core hole than the 4*s* and 4*p* states. I will discuss the interactions within the two-state cluster model including the core spin-orbit coupling, the core-valence electron-electron interactions (aka multiplets), the crystal field. Additional interactions that must be included for a more accurate spectral shape simulation, including (a) a third configuration, (d) additional 4th and 5th configurations, non-local screening, configuration-interaction between core levels and the band structure.

Theory **Wednesday, 15th April, 12:10**

From Core to Valence States: a Comprehensive Experimental and Theoretical Photoelectron Spectroscopy Study of Proteinogenic Amino Acids

Shiyang (Ann) Lu[1], Anna Regoutz[1], Laura Ratcliff[2]

[1]University of Oxford, Oxford, United Kingdom. [2]University of Bristol, Bristol, United Kingdom

Amino acids (AAs) are fundamental building blocks of life. In the solid state, AAs are of considerable scientific and technological interest due to their widespread use in the food and pharmaceutical industries. Despite this, most spectroscopy studies focus on gas-phase species or surface adsorbates, while crystalline AAs remain underexplored, largely because of experimental challenges associated with radiation damage.

A detailed understanding of chemical bonding in solid-state AAs, encompassing both intra- and inter-molecular interactions, is nevertheless of great interest. Photoelectron spectroscopy provides access to this information, however, spectra are often too complex and difficult to interpret. This motivates a combined experimental-theoretical approach, in which density functional theory (DFT) is used to calculate simulated spectra based on known crystal structure. Composed primarily of light elements, readily available in high purity and crystallinity, and exhibiting systematic variation in key chemical motifs, proteinogenic AAs constitute an ideal model system for validating the robustness of such an integrated experiment-theory framework.

Photoelectron spectroscopy measurements, including core, semi-core, and valence states, form the experimental basis with a particular focus on mitigation of radiation damage. Calculated relative core binding energies show excellent agreement with experiment and enable reliable assignments. Projections of the density of states provide insight into the influence of local coordination and extended crystal structure, yielding a systematic understanding of the electronic structure and bonding in solid-state AAs.

This work presents a computationally efficient strategy for unlocking the information encoded in experimental photoelectron spectra and lays the foundation for a broader application of theory-assisted photoelectron spectroscopy.

Theory **Wednesday, 15th April, 14:15 (INVITED)**

Assoc Prof Atsushi Hariki
Department of Physics and Electronics, Osaka Metropolitan University, Japan

Atsushi Hariki is an Associate Professor at Osaka Metropolitan University. His research focuses on the theory of X-ray spectroscopies in correlated electron systems, including d- and f-electron compounds. A current focus is the development of computational methods that combine first-principles electronic structure calculations with many-body approaches such as density functional theory and dynamical mean-field theory, enabling high-accuracy simulation of hard X-ray photoelectron spectroscopy and related spectroscopies.

X-ray Photoemission Spectroscopy Constrained DFT+DMFT Modeling of Correlated Materials

Atsushi Hariki

Department of Physics and Electronics, Osaka, Japan

Accurate theoretical modeling of electronic structures in correlated materials remains a major challenge. Density functional theory (DFT) combined with dynamical mean-field theory (DFT+DMFT) has emerged as a standard approach for describing such systems; however, its practical implementation can face ambiguities, for example due to the necessity of introducing a double-counting correction. In this work, we demonstrate that photon-energy-dependent X-ray photoemission spectroscopy (XPS) provides experimental constraints that largely reduce these ambiguities in DFT+DMFT modeling.

We demonstrate the capability of this approach for selected 3*d* transition-metal compounds including bilayer nickelates, and for 5*f* uranium compounds (UTe_2, UCd_{11}, UGa_2, UB_2) (1-3). The resulting DFT+DMFT models allow us to quantify the valence configuration histograms of the correlated *d* and *f* shells, and further to access time-dependent charge and spin dynamics. Strong charge-transfer effects and orbital-dependent correlations are revealed in the bilayer nickelates. In the uranium compounds, the localization of 5*f* electron is quantified based on their charge correlation functions.

Particular focus is placed on interpreting the pronounced material dependence of satellite features in core-level photoemission spectra among these compounds. Within the DFT+DMFT models, we systematically disentangle the key factors for these features, including valence fluctuations (mixed, intermediate valence), final-state interference and screening effects, and hybridization with a continuum bath beyond nearest-neighbor ligands.

1. D. Takegami *et al.*, Phys. Rev. B **111**, 165101 (2025).
2. A. Marino *et al.*, Phys. Rev. Research **6**, 033068 (2024).
3. M. Sundermann *et al.*, Phys. Rev. Research **7**, 043195 (2025).

Theory Wednesday, 15th April, 14:40

Anisotropic Recoil Effects in Hard X-ray Graphene C 1s Photoemission

Simone Ritarossi[1], Alice Apponi[1], Orlando Castellano[1], José Lorenzana[2], Domenica Convertino[3], Camilla Coletti[3,4], Francesco Offi[1], Tien-Lin Lee[5], Alessandro Ruocco[1]

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Phonon recoil in HAXPES has been studied both experimentally and theoretically in carbon-based anisotropic systems such as graphite (1,2), yet monolayer graphene poses distinct challenges: the purely 2D phonon structure activates flexural modes absent in the bulk, and the intrinsic electronic asymmetry of sp^2 carbon must be carefully disentangled from the phonon-driven recoil response before any quantitative modelling is meaningful.

To address this, C 1*s* spectra of monolayer graphene (CVD-grown on Cu, transferred onto a Ni TEM grid) were acquired at the I09 beamline of Diamond Light Source (3) using a VG Scienta EW4000 HAXPES analyzer at photon energies of 0.8, 4, and 8 keV and at normal and grazing emission angles, providing a dataset with controlled angular and energy sensitivity across a wide recoil-momentum range.

We model the data within the Fujikawa–Takata cumulant framework (1,2), constructing a graphene-specific anisotropic vibrational density of states with cutoff energies constrained by first-principles phonon calculations. The key advance is an explicit electronic convolution strategy: a photon-energy-independent Doniach–Šunjić lineshape, anchored to the near-recoilless 0.8 keV data, is convolved with the phonon recoil kernel, yielding parameter-free predictions that quantitatively reproduce the angle-dependent recoil shifts and line broadenings at 4 and 8 keV, with residuals below 10 meV at 8 keV.

(1) Y. Takata et al., Phys. Rev. B 75, 233404 (2007).
(2) T. Fujikawa et al., J. Electron Spectrosc. 151, 170 (2006).
(3) T.-L. Lee & D. A. Duncan, Synchrotron Radiation News 31, 16 (2018).

Theory Wednesday, 15th April, 14:55 (INVITED)

Prof Dr Ján Minár
University of West Bohemia, Czech Republic

Prof. Minár leads the Quantum and Advanced Materials team at NTC. His research focuses on the electronic structure of solids and low-dimensional systems, electron spectroscopy (ARPES, SARPES), and the development of first-principles methods for strongly correlated and quantum materials. He also contributes to advancing theoretical tools for understanding magnetic and electronic properties of complex materials by soft and hard X-ray ARPES.

One-step Photoemission Model: Core Levels to Valence Bands in Quantum Materials

Jan Minar

New Technologies-Research Centre, University of West Bohemia in Pilsen, Pilsen, Czechia

Angle-integrated and angle-resolved photoemission in the soft and hard X-ray regimes have become essential tools for investigating the bulk properties of various materials. In practice, enhanced bulk sensitivity can be achieved through threshold photoemission. To accurately replicate experimental results, key effects such as matrix elements, photon momentum, phonon excitations, and lattice vibrations must be properly accounted for. In this work, we present a generalized one-step photoemission model implemented within the Munich SPR-KKR program package. This framework coherently describes photoelectron excitation, transport to the surface, and emission into the vacuum. Moreover, it is applicable across a wide photon energy range, from a few electron volts to over 10 keV. The model's ability to incorporate correlation and thermal effects, in combination with the coherent potential approximation method, is demonstrated through various examples. The analysis of ARPES data in terms of three-dimensional electron dispersions typically relies on the free-electron approximation for the photoemission final states. However, at high excitation energies, these final states can become significantly more intricate, involving multiple Bloch waves with distinct out-of-plane momenta. The interpretation and related treatment for multiband final states will be discussed. Special emphasis is placed on the implementation of X-ray photoelectron diffraction, including the treatment of Kikuchi fine structure and circular dichroism in angular distributions for the core levels. Furthermore, the model has been instrumental in confirming the altermagnetic lifting of Kramers spin degeneracy, a key feature of altermagnetism, which represents a novel class of magnetism with significant implications for both fundamental research and technological applications.

Methods Wednesday, 15th April, 15:50

Soft X-rays, Hard Questions: Identifying Band Character in Quantum Materials with ARPES

Jessica McChesney

Argonne National Laboratory, Lemont, United States

We highlight the Intermediate Energy X-ray (IEX) beamline 29-ID at the Advanced Photon Source (APS), optimized for SX-ARPES with variable polarization, a near–magic-angle geometry that minimizes broadening and footprint, sub-10 K six-axis cryogenic manipulation, and integrated x-ray absorption (total/partial electron yield) alongside photoemission. The APS Upgrade extends the accessible photon-energy range to hν ≈ 184–2000 eV with increased flux, strengthening opportunities for bulk and buried-interface studies. I'll present several examples illustrating how the photon-energy dependence and polarization can be used to disentangle band character. For instance, in the heavy-fermion compound Ce2RhIn8, SX-ARPES suppresses problematic surface contributions and yields near-constant-kz momentum cuts, clarifying bulk Fermi-surface signatures in the low-temperature hybridized regime while revealing strong matrix-element effects that motivate matrix-element-aware modeling. In addition, circular dichroism SX-ARPES can be used to investigate the topology of the band structure. In the nodal-line semimetal ZrSiS, circular dichroism SX-ARPES reveals ~30% dichroism for both Dirac bands near the Fermi level and deeper valence states, with sign reversals across crystallographic mirror planes.

Methods **Wednesday, 15th April, 16:05**

Towards Multi-Modal and Operando: Simultaneous Photoemission and Structural Measurements of Gas–Solid Catalysts near 1 bar at Beamline P22

Fernando García Martinez[1], Wieland Corts[2], Steffen Tober[1], Silvan Dolling[1], Heshmat Noei[1], André Rothkirch[1], Hans-Georg Steinrück[2], Martin Beye[3], Christoph Schlueter[1]

[1]Deutsches Electronic Synchrotron DESY, Hamburg, Germany. [2]Forschungszentrum Jülich, Jülich, Germany. [3]Stockholm University, Stockholm, Sweden

Large-scale industrial processes, such as the Haber-Bosch synthesis, depend heavily on gas-solid catalysis. Understanding the interplay between the gas phase and the catalyst surface is key to improving such processes, requiring techniques capable of probing this interface close to industrial conditions ($\geq$1 bar). With this aim, operando techniques have expanded rapidly in recent years, enabling studies of catalysts under realistic conditions with unprecedented detail.

The POLARIS instrument, a fruitful collaboration between the Nilsson/Beye group (Stockholm University) and beamline P22 (PETRA III, DESY), pushes the pressure limits of ambient pressure hard X-ray photoemission spectroscopy (AP-HAXPES). The instrument employs a virtual cell configuration, flowing gas towards the catalyst surface and creating a highly localized pressurized area (pressure $\approx$ 1 bar, volume $<$ 1 mm^3). Hard X-rays penetrate this cell, generating energetic photoelectrons that are collected by a small aperture towards the electron analyzer placed in close proximity to the sample (gap and diameter $<$ 50 µm).

Chemical reactions occur at the catalyst surface. Grazing-incidence geometry is hence required to retain surface sensitivity during AP-HAXPES measurements, resembling structural techniques such as X-ray reflectivity (XRR) and small angle X-ray scattering (SAXS). This similarity can be exploited by placing an X-ray-transparent window in the reactor and an X-ray detector downstream, allowing to simultaneously measure the scattered beam under identical conditions to AP-HAXPES. Early results from this recently commissioned multimodal setup will be discussed, illustrating the potential of combining chemical and structural measurements under operando conditions for materials science and catalysis.

Methods **Wednesday, 15th April, 16:20**

The APE-TX Project: a New HAXPES Beamline at the Elettra 2.0 Synchrotron

Federico Motti[1,2], Jun Fujii[2], Andrea Fondacaro[2], Davide Benedetti[2], Gian Marco Pierantozzi[2], Giovanni Vinai[2], Giorgio Rossi[2,3], Piero Torelli[2], Giancarlo Panaccione[2]

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Synchrotron beamlines combining soft and hard x-rays for electron spectroscopies (HAXPES, XPS, soft X-ray ARPES and XAS) are rare. Existing examples are the I09 beamline at the Diamond Light Source, and the EMIL beamline at Bessy. In both cases two different undulators generate the soft and hard X-rays, that can be eventually recombined in a single end-station.

The Elettra synchrotron was originally optimized for generation of soft X-ray radiation for spectroscopy experiments. The forthcoming upgrade to the diffraction-limited storage ring, Elettra 2.0, will significantly increase brilliance in the tender-X-ray range, making these energies increasingly attractive. This talk reviews the status of the APE-TX beamline project at Elettra 2.0.

The beamline has the ambitious aim to channel the wide range of photon energies (0.5 to 6 keV) emitted from a single undulator source towards two different end-stations. The optical layout, designed in collaboration with the optics group of the Photon Factory (Tokyo, Japan), allows channeling tender and soft X-rays through the same optical path, with minimal changes to switch the energy range. Two complementary monochromator technologies are employed: gratings for soft X-rays, and crystal diffractors for tender X-rays. Both monochromators will be mounted on translation stages, that allow to select which optical elements will intersect the photon beam. One end-station will be dedicated to photoemission experiments (XPS and HAXPES) in ultra-high-vacuum, the second to in-operando studies at ambient pressure (including XAS).

Methods **Wednesday, 15th April, 16:35**

Multimodal Measuring System for Chamberless HAXPES and XRD at the BL46XU Beamline of SPring-8

Okkyun Seo, Takeshi Watanabe, Yasumasa Takagi, Satoshi Yasuno, Tappei Nishihara

JASRI, Sayo, Japan

Hard X-ray photoelectron spectroscopy (HAXPES) is a powerful, bulk-sensitive tool for analyzing electronic structure, capable of resolving features down to tens of nanometers. While traditional X-ray Diffraction (XRD) provides structural data at micrometer scales, combining these techniques has historically been limited by environmental constraints. Here, we present a novel instrumentation setup at the SPring-8 BL46XU beamline designed for simultaneous, chamberless HAXPES and XRD using a single hard X-ray source.

By operating outside a vacuum chamber, this system enables the concurrent analysis of crystal structure, chemical states, and electronic properties under ambient atmospheric conditions. To mitigate signal degradation from atmospheric scattering, we implemented a localized Helium gas injection system, significantly reducing background noise and enhancing the HAXPES signal-to-noise ratio. This integrated approach bypasses the limitations of conventional vacuum-based XPS, offering a new experimental paradigm for the comprehensive characterization of materials in their natural or operative environments.

Methods **Wednesday, 15th April, 16:50**

HAXPES at 4th Generation Synchrotron

Jean-Pascal Rueff

Synchrotron SOLEIL, St Aubin, France

The advent of 4th generation synchrotrons will profoundly renew the HAXPES field of research in the near future. Based on more than 10 years of experience of HAXPES for advanced materials studies at the GALAXIES beamline (1) of the SOLEIL Synchrotron, including investigation of quantum materials (2), energy related materials (3) or liquid phases (4), we will address the benefits and challenges of HAXPES offered at these new facilities. The discussion will be illustrated by recent results obtained at the GALAXIES beamline, especially in the context of the forthcoming SOLEIL II upgrade.

(1) Rueff et al., J. Synchrotron Rad. **22**, 175 (2015)
(2) Raji et al., *Advanced Functional Materials* ***34*** 2409930 (2024)
(3) Atkins et al., Advanced Energy Materials **12**, 210268 (2021)
(4) Mosaferi et al., J Am. Chem. Soc. ***146,*** *9836 (2024)*

Application II Energy Thursday, 16th April, 09:00 (PLENARY)

Dr Christoph Schlueter
Beamline P22, Deutsches Elektronen-Synchrotron (DESY), Germany

Christoph Schlueter is a physicist specializing in hard X-ray photoelectron spectroscopy (HAXPES) and synchrotron-based materials characterization. He earned his PhD from Hamburg University in 2013 while based at ESRF's ID32 beamline, followed by postdoctoral research at Diamond Light Source's I09. Since 2013, he has led P22, DESY's dedicated HAXPES beamline at PETRA III. The beamline hosts four specialised endstations (HAXPES, HarMoMic, HAXPEEM, POLARIS), each advancing the state of the art in photoelectron spectroscopy and enabling research across fields from in-situ catalysis to quantum materials. His work focuses on developing techniques to probe electronic and chemical properties of complex systems.

P22 at PETRA III: A Versatile Platform for Advanced HAXPES Studies

Christoph Schlueter

DESY, Hamburg, Germany

The P22 undulator beamline at PETRA III is a dedicated platform for advanced hard X-ray photoelectron spectroscopy (HAXPES), providing a versatile environment for probing the electronic and chemical structure of complex materials under realistic conditions. The beamline integrates four complementary endstations covering a broad range of experimental approaches.

A high-resolution hemispherical analyzer serves as a workhorse for operando device characterization, depth profiling, and quantitative chemical analysis. The ambient-pressure system POLARIS enables studies of catalytic processes under industrially relevant conditions. The hard X-ray momentum microscope (HarMoMic) provides wide-field access to band dispersions and photoelectron diffraction, while the HAXPEEM instrument enables spatially resolved chemical analysis.

These capabilities have enabled studies of buried functional interfaces in microelectronic devices, operando investigations of catalytic reactions, and momentum-resolved access to bulk electronic structure. Building on this foundation, P22 is evolving towards a more integrated and scalable HAXPES platform, with increasing emphasis on standardized workflows, high-throughput operation, and industrial access.
Since the start of user operation in 2018, P22 has supported a broad international community and produced over 120 publications, establishing its role as a key facility within the global HAXPES landscape.

Application II Energy **Thursday, 16th April, 09:45 (INVITED)**

Prof Louis Piper
WMG, University of Warwick, United Kingdom

Louis Piper is the Professor of Battery Innovation and heads the Battery Materials and Cells group at WMG, the University of Warwick, which includes AMBIC prototype pilot line. He has published over 200 publications and has various projects with industry partners and government agencies. He co-leads the Faraday Institution's Lithium ion: Enhancing and Accelerating Performance – LEAP consortium project. His research areas have covered various functional materials for energy harvesting, storage and efficiency, employing a range of x-ray and related techniques. He is currently focused on accelerating the development of battery materials, combining real formats and advanced characterization. Physics PhD (Warwick), Post-Doc (Boston University), tenure track to Full Prof. (Binghamton University, State University of New York), he joined WMG in 2020.

Oxygen Redox in Batteries: The Hole Picture

Louis Piper

University of Warwick, Coventry, United Kingdom

Layered transition metal oxides used in rechargeable alkali-ion batteries are commonly described within an ionic redox framework, where charge compensation proceeds via formal transition metal oxidation. At high states of charge, however, anomalous capacity and spectroscopic signatures have frequently been interpreted as oxygen redox, where oxygen–oxygen dimerization or trapped molecular O_2 are among possible candidates.

(1) Recent studies have cast doubt on trapped O_2 dimers as the source of electrochemistry, e.g., Ref. (2) and prompts the question: how is oxygen participating in the redox mechanism?

Here, I will summarise how HAXPES and resonant photoemission have contributed to the discussion on the nature of oxygen redox. Using resonant photoemission spectroscopy combined with DFT+DMFT calculations it is possible to directly study the depopulation of the orbitals during (de) intercalation, which provides direct spectroscopic evidence for ligand-hole character in late transition metal oxides at high oxidation states.(3) The redistribution of spectral weight and evolution of hybridised O 2*p* – late TM 3*d* states are consistent with a negative charge transfer description, where charge compensation occurs via oxygen-derived ligand holes rather than discrete O–O bond formation. This "hole picture" reconciles oxygen participation in redox with established electronic structure models of correlated oxides. Beyond batteries, these results highlight the importance of bulk-sensitive photoemission and resonant probes in disentangling intrinsic electronic structure from defect-driven surface phenomena in transition metal oxides.

(1) Nature Reviews Materials 7, 522–540 (2022) (2) Joule 9, 101775 (2025); (3) arXiv:2505.01251 - accepted in press (2026)

Application II Energy Thursday, 16th April, 10:10

From Surface to Bulk: Chemical and Electronic Structure Evolution of Delithiated LiNi0.8Mn0.1Co0.1O2 Electrodes - Insights Into pSEI Formation and Redox Mechanisms with Lab-Based Coupled Soft and Hard XPS

Yanis Jugie[1], Roberto Fantin[2], Mohammed Raghibi[2], Ambroise Van Roekeghem[1], Renaud Bouchet[2], Anass Benayad[3]

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Layered transition metal oxides $Li_xNi_wMn_yCo_zO_2$ (NMCwyz, w+y+z=1) represent state-of-the-art positive electrode materials for Li-ion batteries. In these electrodes, charging occurs through Li^+ deintercalation and redox reactions, producing a strong stoichiometric gradient between the surface and the bulk during electrochemical cycling. Investigating the redox process requires a non-destructive approach that probes changes in the local electronic structure of the transition metals and oxygen atoms during cycling at the sub-nanometer scale. X-ray photoelectron spectroscopy (XPS) is a well-established technique to study the redox process and the positive electrode Solid Electrolyte Interphase (pSEI) in $Li_xNi_wMn_yCo_zO_2$ materials. However, interpreting the final state electronic structure and determining the formal oxidation state of the metal atoms upon charge remain challenging due to the high surface sensitivity of XPS and the overlap of Auger features with transition-metal core levels when using soft X-ray energies. In this study, combined soft and Hard X-ray photoelectron spectroscopy (resp. XPS, Al Kα, 1.5 keV and HAXPES, Cr KΓ, 5.4 keV) were employed to study the impact of lithium disinsertion on the electronic structure of $Li_xNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ electrodes, with $x \approx 1, 0.7, 0.4, 0$. Within the first 15 nm, we elucidate the respective contributions of metal and oxygen species to the charge-compensation mechanism. Furthermore, by employing reference metal oxides with well-established formal oxidation states, we develop a protocol to quantify surface and bulk contributions using laboratory-derived HAXPES sensitivity factors for delithiated states during the first charge. These results are analyzed with respect to the pSEI formation and its influence on surface stoichiometry evolution.

Application II Energy Thursday, 16th April, 10:25

Dynamic Interphases in Halide Solid-State Batteries Revealed by Operando XPS: Open Questions for HAXPES

Rosalía Cid Barreno, Maider Elosua, Pierre Lannelongue, Miren de Lasén, Pedro López-Aranguren

CIC energiGUNE, Vitoria-Gasteiz, Spain

Unlocking electrochemical interfaces is key to advancing solid-state batteries, yet the decisive chemistry often occurs in buried, fast-evolving interphases that are hard to access without artifacts. XPS is a cornerstone for Solid Electrolyte Interphase (SEI) analysis, but conventional ex-situ workflows can miss transient intermediates and, in solid-state systems, Li | electrolyte interfaces are frequently disrupted during sample preparation.

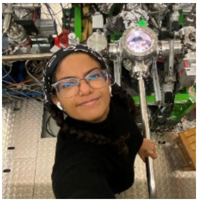
Here we deploy virtual-electrode operando XPS (OpXPS) to electrodeposit Li directly onto a halide solid electrolyte ($Li_3YCl_2Br_4$, LYCB) inside the XPS, enabling real-time tracking of interphase formation from the earliest stages. OpXPS captures rapid formation of LiX (X = Cl, Br) together with strong changes in Y-containing species (reduction and re-oxidation), followed by time-dependent redistribution of species consistent with progressive stratification. In the final state accessible with XPS LiX dominates the outer region while Y-based products become increasingly buried. The apparent growth rate slows after an initial burst, consistent with an electron-transport limitation through a mixed ionic–electronic conducting interphase.

Electrochemical impedance spectroscopy (EIS) and distribution of relaxation times (DRT) link chemistry to function: under static contact the interfacial resistance continues to rise, whereas stripping/plating accelerates convergence toward a more stable response, supporting a self-limiting layered architecture that suppresses electron leakage while maintaining Li^+ transport.

Because lab XPS is depth-limited, key questions remain about buried chemical states and long-time evolution beneath plated Li. We discuss how photon-energy-dependent HAXPES could non-destructively map chemistry vs depth, quantify the electron-blocking layer, and reveal hidden products, opening clear opportunities for collaboration toward realistic halide solid-state cells.

Application II Energy Thursday, 16th April, 11:10 (INVITED)

Dr Prajna Bhatt
Istitutio Officina dei Materiali, Consiglio Nazionale
delle Ricerche (CNR-IOM), Italy



Prajna Bhatt is a postdoctoral fellow at Istitutio Officina dei Materiali in the Consiglio Nazionale delle Ricerche (CNR-IOM) in Trieste, Italy since 2025. Her research activity focuses on the development of a new laboratory-based hard X-ray photoelectron spectroscopy (HAXPES) system, APE-TX. Her research also focuses on the electronic properties and buried interfaces of oxides, hydrides and piezoelectric systems, using synchrotron radiation and conventional X-ray source XPS. She obtained her MSci in Natural Sciences specialising in Inorganic and Materials Chemistry in 2017 with Prof. Anna Regoutz (now at the University of Oxford, UK) and her from PhD in 2025 from University College London, UK, carrying out her research with Prof. Robert Palgrave.

Lifetime Effects and Satellites in the Photoelectron Spectrum of Platinum Metal

Prajna Bhatt[1], J. J. Gutiérrez Moreno,[2], L. E. Ratcliff[3,4], A. A. Riaz[5], C. M. L. André[6,7], S. Liu[7], R. G. Palgrave[5], A. Gloskovskii[8], C. Schlueter[8], P.K. Thakur[9], T.-L. Lee[9], A. Regoutz[7]

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London, United Kingdom. [6]Universit´e Paris-Sacla, Paris, France. [7]University of Oxford, Oxford, United Kingdom. [8]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany. [9]Diamond Light Source, Harwell, United Kingdom

Platinum (Pt) is a vital transition metal that is most notably known for its use in catalysis. An analytical technique commonly used on Pt and its compounds is X-ray photoelectron spectroscopy (XPS), which probes the surfaces of these materials and allows for studies of chemical states and electronic structures. However, few works in the literature provide information on the origin and nature of satellite features that are prominent in the photoelectron core-level spectra and of a detailed understanding of valence states in Pt. Due to this, spectra can at-times be misinterpreted in the literature. The present work combines high-resolution soft and hard XPS (SXPS and HAXPES) with (high-energy) reflected electron energy loss spectroscopy (R(H)EELS) and a multi-tiered ab initio theoretical approach, including density functional theory and many-body perturbation theory (G_0W_0), to disentangle the complex set of experimentally observed features attributed to the generation of plasmons and interband transitions. This combined experiment-theory strategy allows for the reporting and assignment of previously undocumented satellite features and aids in improving our understanding of platinum's electronic structure. Furthermore, studies of the valence band uncovered how different theoretical approaches are able to describe the experimentally obtained spectra. This work aims to provide a foundation for future studies into platinum-based mixed-metal systems and improve our understanding of the pure Pt metal system. It also encourages the study of other elements, done in a similar manner previously for tungsten and titanium.

Application II Energy **Thursday, 16th April, 11:35**

The Hidden Surface Transformation That Limits Ni-Rich Li-Ion Batteries

Galo Paez Fajardo[1,2], Gerard Bree[1,2], Eleni Fiamegkou[1,2], Ieuan D. Seymour[3], Hrishit Banerjee[4,5], Israel Temprano[6,7], Pardeep K. Thakur[8], Tien-Lin Lee[8], Louis Piper[1]

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Instability of the interface between Ni-rich cathode surface and electrolyte limits how much energy rechargeable alkali-ion batteries store per cycle.

The industrial method to circumvent these interface instabilities includes narrowing the voltage window, leaving up to ~30% of the theoretical capacity inaccessible, impacting efforts on advanced energy density devices and next-generation batteries. The interface instabilities are commonly described as rock salt phases, (1, 2) yet their chemical nature, formation pathway, and evolution during long-term cycling remain open questions.

Here, I will summarise how HAXPES, together with complementary X-ray probes and first-principles quantum approaches, has advanced the discussion of rock-salt formation and stability in industrially relevant, machine-made electrodes and format cells (3–5). By integrating operando changes with ex-situ HAXPES, soft XAS, and DFT+DMFT, I will detail how the interfacial phases transform with cycling. An early, Li-rich rock-salt-like surface phase acts as an "open gate" for Li transport, but with cycling it densifies into a Li-poor rock-salt phase that becomes a "closing gate," driving Li "traffic jams" and faster capacity fade. These results highlight how photoemission, integrated with complementary methods, can disentangle technologically relevant surface phenomena and inform voltage-operating protocols that could safely access more capacity and improve device-level performance.

(1) *Adv. Mater.* 2025, 37, 2419253;
(2) *Chem. Rev.* 2025, 125, 20, 9774–9806;
(3) *ACS Energy Lett.* 2023, 8, 12, 5025–5031;
(4) *PRX Energy* **3**, 013004;
(5) *ACS Energy Lett.* 2025, 10, 3, 1313–1320

Application II Energy Thursday, 16th April, 11:50

Investigating the Contributions of Solid Electrolyte Interphases to the Electrochemical Stability Window of Aqueous Electrolytes in Li-Ion Batteries

Conor Phelan, Jasper Singh, Erik Erik Björklund, Zachary Goodwin, Robert Weatherup

Department of Materials, University of oxford, Oxford, United Kingdom

The growing deployment of intermittent renewable energy, rapid expansion of electric vehicles, and increasing demand for portable electronics have intensified the need for safe, reliable, and cost-effective energy storage technologies. Aqueous electrolyte lithium-ion batteries offer a compelling alternative to conventional organic systems due to their intrinsic safety, lower cost, and higher ionic conductivity. However, their commercial viability has been constrained by the narrow electrochemical stability window (ESW) of water, which decomposes at extreme potentials.

Recent advances demonstrate that this limitation can be mitigated using highly concentrated Water-in-Salt Electrolytes (WiSEs). These formulations alter the bulk solvation structure, promote electrode passivation, and modify ion transport and reaction kinetics, collectively suppressing water decomposition at both electrodes. With careful optimization, ESWs exceeding 3.5 V have been achieved, enabling stable cycling of $LiMn_2O_4$ (LMO) vs. $Li_4Ti_5O_{12}$ (LTO) full cells.

To uncover the mechanisms responsible for suppressed water breakdown, we combine depth-resolved X-ray Photoelectron Spectroscopy (XPS). Complementary Classical Molecular Dynamics simulations, along with Nuclear Magnetic Resonance (NMR) and Raman spectroscopy, probe the solvation environment and degradation pathways that govern cathode/solid-electrolyte interphase formation.

Application II Energy **Thursday, 16th April, 12:05**

Impact of PEAI Passivation on Buried Interfaces in PSCs Probed by Operando HAXPES

Rahul Mahavir Varma[1], Karen Radetzky[1,2], Fredrik OL Johansson[1], Soham Mukherjee[1], Ute Cappel[1,2], Håkan Rensmo[1,2]

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In this presentation, we demonstrate how synchrotron-based photoemission spectroscopy, particularly hard X-ray photoelectron spectroscopy (HAXPES), can be employed to investigate interfacial chemical reactions, energy band alignment, and ion migration in complete perovskite solar cell (PSC) stacks. To selectively probe the various interfaces within the PSC, we optimized PSC devices by systematically reducing the thickness of gold contact layer and hole transport layer (HTL) while preserving the functionality of PSC device. This approach enables depth-resolved access to buried junctions without compromising device operation.

The HAXPES measurements were first used to elucidate the intrinsic interfacial chemistry and chemical interactions between the $FAPbI_3$ and the spiro-OMeTAD HTL. We observed clear sign of chemical modification and ion migration happening at the $FAPbI_3$/spiro-OMeTAD interface. The comparative analysis of passivated and non-passivated PSC demonstrates that phenethylammonium iodide (PEAI) effectively suppresses undesirable interfacial reactions and stabilizes the perovskite surface.

Operando HAXPES experiments (I09 beamline, Diamond light source) were subsequently performed under light illumination to probe working devices in real time. These measurements provide direct insight into light induced chemical modifications, possible ion redistribution at the interfaces, and energy band alignment by tracking potential drops across different layers. Thereafter, the applied bias experiments (in dark) were performed to assess whether electrically driven operation induces similar interfacial changes as illumination.

Overall, this work provides insights into the chemical and electronic evolution of critical PSC interfaces under operating conditions. The findings offer valuable guidelines for mitigating interfacial degradation and advancing the design of more stable perovskite solar cells.

Application II Energy **Thursday, 16th April, 12:20**

Zinc depletion at the ZnFe2O4 (1 1 1) single crystal surface: X-ray spectroscopy (NEXAFS and XPS) experiments and computer simulations

Pilar Ferrer[1] Charlotte A Hall[1], David C Grinter[1], Jonas Sandermann[2], Bo Brummerstedt Iversen[2], Róger A Bennett[3], Georg Held[1], Ricardo Grau-Crespo[3,4]

[1]Diamond Light Source, Didcot, United Kingdom. [2]Center for Sustainable Energy Materials, Aarhus University, Aarhus, Denmark. [3]Department of Chemistry, University of Reading, Reading, United Kingdom. [4]School of Engineering and Materials Science, Queen Mary University of London, London, United Kingdom

Near-Edge X-ray Absorption Fine Structure (NEXAFS) and conventional X-ray Photoelectron Spectroscopy (XPS) are techniques for probing the surface and near-surface regions of materials, being complementary to the Hard X-ray photoelectron spectroscopy (HAXPES) technique.

In this study, we investigate the surface composition of zinc ferrite ($ZnFe_2O_4$) (1 1 1) single crystals obtained by different preparation methods, combining both experimental and computational techniques (Applied Surface Science 713, 164253, 2025). Angle-resolved NEXAFS experiments were done to improve the surface sensitivity, together with depth-profiled XPS to complement the measurements. Analyses reveal that ultra-high vacuum (UHV) annealing leads to Zn depletion and the formation of an iron-rich (1 1 1) surface, whereas annealing in an O_2 atmosphere preserves a bulk-like $ZnFe_2O_4$ surface composition. Detailed examination of the Fe 2*p* photoemission and Fe L-edge absorption signals shows a clear difference in iron oxidation states and cation distributions under these preparation conditions. UHV annealing yields a mixed Fe^{2+}/Fe^{3+} state and a cation distribution like that of a magnetite (Fe_3O_4), while oxygen annealing results in Fe^{3+} ions, predominantly in octahedral coordination, consistent with the expected structure of $ZnFe_2O_4$. These study highlights the critical influence of preparation environment on the surface chemistry and electronic structure of zinc ferrite.

Application II Energy Thursday, 16th April, 13:30

Interfacial Chemistry Limits the Stability of Deep Blue Perovskite LEDs Revealed by Operando Characterization

Alessandro Mirabelli[1], Birgit Kammlander[2], Ute Cappel[2], Sam Stranks[3]

[1]University of Cambridge, Cambridge, United Kingdom. [2]University of Uppsala, Uppsala, Sweden. [3]Universityo of Cambridge, Cambridge, United Kingdom

To commercialize lead halide perovskites as light-emitting diodes (LEDs), the operational device lifetime needs to be drastically improved. For this to be achieved, an understanding of degradation behavior under bias is crucial. Herein, we perform operando measurements of the structural, chemical, and electronic changes using synchrotron-based grazing-incidence wide-angle X-ray scattering and hard X-ray photoelectron spectroscopy on full-stack deep blue mixed bromide/chloride lead halide perovskite LEDs. While a clear drop in optoelectronic performance is recorded under electrical bias, the accompanying X-ray scattering data reveals only minor changes in structural properties. However, photoelectron spectroscopy reveals substantial chemical changes at the electron-injecting interface after bias is applied, including the formation of unwanted metallic lead and a new chlorine species that is not in the perovskite structure. These operando approaches give important structural and interfacial perspectives to reveal the degradation mechanisms in these LEDs and highlight the need to address the top electron-injecting interface to realize step-changes in operational stability

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Application II Energy Thursday, 16th April, 13:45

Ligand Donor Number from Potassium X-ray Photoelectron Spectroscopy

Frances Towers Tompkins[1], Lewis Parker[1], Najaat Alblewi[1], Jake Seymour[1], Roger Bennett[1], Robert Seidel[2], Denis Céolin[3], David Duncan[4,5], Kevin Lovelock[6]

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Potassium-ligand interactions, where the ligand can be an anion or a molecule, are fundamental to electrochemical energy storage, biological processes, and organopotassium chemistry. The strength of K^+-ligand interactions is a key metric for the development of potassium-ion battery electrolytes - ligand stripping from K^+ to allow K^+ intercalation at the anode is crucial in potassium-ion battery charging. However, experimental quantification of K^+-ligand interactions remains challenging, as K^+ is spectroscopically quiet; common spectroscopies such as UV-vis and NMR have no K^+ contribution.

We utilise hard and soft XPS to directly probe K^+ in solution. (1) Liquid-jet hard XPS (GALAXIES) and ionic liquid drop hard XPS (I09) to obtain E_B(K 1*s*) for K^+ solvated by solvent (water and propylene carbonate) and anion ((SCN), $(NTf_2)^-$, $(FSI)^-$) respectively. (2) Liquid-jet soft XPS (SOL^{3}PES) and ionic liquid drop soft XPS (lab XPS) to obtain E_B(K 2*p*) for K^+ - the overlap of K 2*p* and C 1*s* demonstrates the importance of hard XPS.

We use E_B(K 1*s*) to produce, for the first time, an experimental K^+-ligand interaction strength scale, called the donor number ($DN_{K\text{-}XPS}$). These E_B(K 1*s*) and therefore $DN_{K\text{-}XPS}$ reflect the electrostatic potential at the K nucleus, V_K, providing an interpretable measure of the K^+-ligand interaction strength. This scale will underpin interpretation of potassium-ion battery electrolyte performance. We will make comparisons of $DN_{K\text{-}XPS}$ to other donor numbers measured using XPS (Li^+, Na^+, Mg^{2+}, Mg^{2+}, Zn^{2+}, Ca^{2+}, Al^{3+}), capturing the importance of metal cation charge and size.

Application II Energy **Thursday, 16th April, 14:00**

Bismuth-Based Photoelectrodes Unveiled by HAXPES: Probing the Contribution of Bi 6*s* and Bi 6*p* to the Valence Band

Freddy Enrique Oropeza[1], K. Hongliang Zhang[2], Jan Philipp Hofmann[3]

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Bismuth-based semiconductors, e.g., $BiVO_4$ and Bi_2CuO_4, have been identified as promising photoelectrochemical (PEC) materials owing to their intrinsic optoelectronic properties, such as band gap, charge-carrier mobility, and band energy positions. These properties are strongly influenced by valence Bi 6*s* and Bi 6*p* states. In this contribution, we will discuss the unique capabilities of HAXPES to probe the intrinsic bulk electronic properties of Bi-based photoelectrodes, using $BiVO_4$ and Bi_2CuO_4 as model systems. By exploiting the increased inelastic mean free path and the relatively high photoionisation cross-sections of *s*-states at high excitation energies, HAXPES enables a direct, bulk-sensitive view of the valence band electronic structure with a strong focus on the Bi 6*s* and Bi 6*p* contributions. Whereas valence band maximum of $BiVO_4$ has a strong contribution from Bi 6*s*–O 2*p* hybrid state, this approach unambiguously reveals that Bi 6*s*–O 2*p* hybrid states are located deeper in the valence band (at ~2.3 eV below E_F) for Bi_2CuO_4, while the valence band maximum retains a predominant Cu 3*d*–O 2*p* character, a finding obscured in conventional soft X-ray studies due to the low cross-section of Bi valence states. Combining resonant photoemission and X-ray absorption, we identify that the low-energy optical absorption arises from localised *d*–*d* transitions, which explains the poor photoresponse at visible wavelengths. Extending this methodology to other emerging Bi-based photoelectrodes will be discussed, highlighting how HAXPES provides a rigorous experimental basis for band engineering and the rational design of efficient, Bi-based PEC devices.

Application II Energy Thursday, 16th April, 14:15

A Depth Resolved Investigation of Hydrogen Uptake in Carbon Based Nanostructures

Orlando Castellano[1,2], Alice Apponi[1,2], Daniele Paoloni[1,2], Francesco Offi[1], Simone Ritarossi[1,2], Luca Cecchini[3,4], Ilaria Rago[4], Gianluca Cavoto[3,4], Francesco Pandolfi[4], Carlo Mariani[3,4], Tien-Lin Lee[5], Alessandro Ruocco[1,2]

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Investigation of hydrogen adsorption in carbon-based material is becoming a fundamental issue in the different fields in which hydrogen storage is of interest. A key question is whether hydrogen uptake is surface limited or extends into the bulk, for example in three-dimensional architectures such as nanoporous graphene (NPG) and carbon nanotubes (CNTs), which combine high surface to volume ratio with finite thickness and the presence of internal surfaces (1,2). To address in-depth hydrogenation, we compared pristine and hydrogenated NPG and CNTs using soft and hard X-ray photoelectron spectroscopy (PES) at the I09 beamline of Diamond Light Source. We tracked the hydrogenation-driven transition from sp2 towards sp3 hybridization in the C 1s core level (3) with increasing depth sensitivity. The hydrogen uptake was quantified by fitting the C 1s line shape and converting the extracted sp3 fraction into a depth profile using a thin-overlayer attenuation model, while accounting for the observed recoil effects at high photon energy. We find that hydrogen chemisorption is predominantly surface-limited in both NPG and CNTs. For NPG, the results are consistent with partial hydrogenation of the first accessible graphene layer. For CNTs, the depth profile indicates hydrogenation of outer shells in multi-walled bundles with limited penetration toward inner walls. These findings suggest that hydrogenation may limit permeability of graphene to atomic hydrogen.

(1) S. Iijima, Nature 354, 56 (1991).
(2) Y. Ito et al. Angew Chem Int Ed 53, 4822 (2014).
(3) D. W. Boukhvalov et al. Physical Review B (77) 035427 (2008).

Atomic and Molecular Friday, 17th April, 09:00 (INVITED)

Dr Tatiana Marchenko
CNRS (French National Centre for Scientific Research), France

Tatiana Marchenko graduated in physics from M.V. Lomonosov Moscow State University in Moscow, Russia. She completed her PhD at the FOM Institute for Atomic and Molecular Physics (AMOLF) in Amsterdam, the Netherlands, under the supervision of Prof. Marc Vrakking, focusing on atoms and clusters in strong laser fields. After several postdoctoral appointments in France, she obtained a permanent research position at the CNRS, the French National Centre for Scientific Research. She is currently a Research Director at the Laboratory of Chemical Physics – Matter and Radiation (LCPMR) in Sorbonne University, Paris, where she works in the group of Dr Marc Simon. Her research focuses on X-ray-induced electron dynamics in molecules in the gas, liquid, and solid phases, with particular emphasis on charge-transfer mechanisms in organic systems.

Charge Transfer in Organic Molecules Probed by Resonant Auger Spectroscopy

Tatiana Marchenko

CNRS, Sorbonne University, Paris, France

Charge transfer (CT) processes, governed by the interplay between electronic and nuclear motion, continue to attract significant attention due to their critical role in a broad spectrum of chemical, biological, and material-related phenomena. In complex systems, steering electronic dynamics with high spatial and temporal resolution demands the initiation of CT at a specific site. This level of selectivity can be achieved through X-ray excitation, which enables atomic-level targeting via core-shell electron transitions.

When a system undergoes dynamic relaxation via emission of Auger electrons or X-ray photons occurring within the lifetime of the core-excited state, typically ranging from a few femtoseconds to the attosecond regime, it becomes possible to probe the underlying electron dynamics of CT processes. Using resonant Auger electron spectroscopy and resonant inelastic X-ray scattering in sulfur-containing systems, we gain insight into electron dynamics unfolding on ultrafast timescales defined by the ~1 femtosecond lifetime of the sulfur 1*s* core hole.

We will discuss two applications of these techniques: the elucidation of charge transfer mechanisms in organic polymers and the observation of charge transfer in aqueous amino acid solutions.

Atomic and Molecular Friday, 17th April, 09:25 (INVITED)

Prof Philip Moriarty
School of Physics & Astronomy, University of Nottingham, United Kingdom

Moriarty's research interests span a range of topical themes in nanoscience: scanning probe microscopy, single atom/molecule manipulation, self-organisation of nanostructured systems, synchrotron-based spectroscopies and techniques, and the machine learning-nanotechnology interface. He also has a keen interest in science education and public engagement (not least via the Sixty Symbols project).

Timing the Escape of a Caged Electron

Connor Fields[1], Aleksandra Foerster[2], Sadegh Ghaderzadeh[1], Ilya Popv[1], Bang Hyunh[3], Filipe Junqueira[1], Tyler James[4], Sofia Alonso Perez[1], David Duncan[1,5], Tien-Lin Lee[5], Sally Bloodworth[6], Gabriela Hoffman[6], Mark Walkey[7], Richard Whitby[6], Malcolm Levitt[6], Brian Kiraly[1], James O'Shea[1], Elena Besley[1], Philip Moriarty[1]

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Australia

Charge transfer is fundamentally dependent on the overlap of the orbitals comprising the transport pathway. This has key implications for molecular, nanoscale, and quantum technologies, for which delocalization (and decoherence) rates are essential figures of merit. In this context, the Ar@C_{60} molecule is an intriguing species: the noble gas atom is encapsulated within the closed-shell fullerene cage and, in the ground state at least, there is minimal mixing of the Ar orbitals with those of the C_{60} cage. As such, one might expect that an intramolecular electronic excitation would couple at best weakly to the surrounding environment. We have applied the core hole clock technique—an energy-domain variant of ultrafast spectroscopy, in this case involving resonant Auger-Meitner de-excitation —to test this hypothesis, i.e., to probe the delocalization rate of a photoexcited electron inside a closed molecular cage. Far from isolating the intracage excited state (Ar $2p^5 4s^1$), the surrounding fullerene is instead a remarkably efficient conduit for electron transfer: we measure characteristic delocalization times of 6.6 ± 0.3 fs and $\lesssim$ 500 attoseconds, respectively, for a 3D Ar@C_{60} film and a 2D monolayer on Ag(111). For the latter, we complement the core hole clock measurements with X-ray standing wave analysis, enabling an accurate determination of the intramolecular position of the argon atom (1). We find a lower rate of charge transfer for adsorption on Pb(111) as compared to Ag(111) (2).

(1) C. Fields *et al., Nature Comms.* **16**, 5062 (2025)
(2) A. Sufyan *et al., Nanosc. Adv.* **7,** 7913 (2025)

Atomic and Molecular **Friday, 17th April, 09:50**

Auger Decay from Doubly Excited Core-Hole States with Sub-Natural Resolution: the Ar K Case

Matjaž Žitnik[1], Mateja Hrast[2], Andrej Mihelič[1], Klemen Bučar[1], Janez Turnšek[1], Ralph Puettner[3], Gildas Goldsztejn[4], Tatjana Marchenko[4], Renaud Guillemin[4], Loic Journel[4], Oksana Travnikova[4], Iyas Ismail[4], Maria-Novella Piancastelli[4], Marc Simon[4], Denis Ceolin[5], Matjaž Kavčič[1]

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HAXPES may be used to collect resonant Auger (RA) emission from core-excited states. The method offers a possibility to isolate contributions of different atomic resonances to the absorption spectrum with better sensitivity than the resonant inelastic X-ray emission (RIXS) and, for doubly excited states (DESs), this potential has not been investigated yet. To demonstrate the options, we have studied the $KM_{23}{-}L_{23}L_{23}M_{23}$ RA emission from the $1s^{-1}3p^{-1}nln'l'$

DESs in argon. We also present a new interference scheme that can significantly disturb the separation of absorption signal pertaining to DES from the underlying core-hole electron continuum even if the DES signal is clearly separated in the RA electron yield. Namely, the K– $L_{23}L_{23}$ RA decay of the $1s^{-1}3p^{-1}nln'l'$ state in Ar was found to interfere with a weak non-resonant process that converts the $1s^{-1}\epsilon p$ low-energy electron continuum to the $2p^{-2}3p^{-1}nln'l'\epsilon(s,d)$ high-energy continuum. This non-resonant process involves three active electrons and is driven by a combination of K – $L_{23}L_{23}$ shake-up Auger decay of $Ar^{+}1s^{-1}$ ion and 1s photoelectron recapture. It turns out that at 16.5 eV above the K ionization threshold of argon, one per thousand of K – $L_{23}L_{23}$ decays is redirected from Ar^{2+} to Ar^{+} decay channel by such Auger shake-up assisted photoelectron recapture. In general, the attempts to separate the resonant part of photoabsorption cross section from the underlying continuum have limited accuracy as soon as the two parts interfere in at least one of the decay channels.

Atomic and Molecular **Friday, 17th April, 10:20 (INVITED)**

Dr Ralph Püttner
Fachbereich Physik, Freie Universität Berlin, Germany

Dr. Ralph Püttner graduated in physics at the Leibnitz-Universität Hannover, Germany, in 1993. In 1998 he received his PhD from the Freie Universität Berlin, Germany under the supervision of Prof. Günter Kaindl working on the field of soft X-ray photoabsorption on atoms and small molecules in the gas phase. After a post-doc position at the University of Oulu, Finland he returned to the Freie Universität Berlin and obtained a permanent research position in 2001. He works on atoms and molecules in the gas and the liquid phase using soft- and hard X-ray spectroscopic tools at both Synchrotron radiation facilities and Free electron lasers.

Electron Spectroscopy of Isolated and Solvated Atoms using Hard X-ray Synchrotron Radiation

Ralph Püttner

Freie Universität Berlinl, Berlin, Germany

Hard X-ray photons provide access to deep core holes in isolated and solvated atoms and molecules, enabling the investigation of new effects.

We present an experimental approach that enables time-resolved synchrotron radiation experiments on a time scale of several 100 attoseconds. This concept is based on decay cascades of core-excited or core-ionized states, with Auger decay serving as the probe. In this study, we investigate the recapture process of slow photoelectrons during Kr $2p_{1/2}$ Auger decays. The Kr $2p_{1/2}$ core holes are produced either by direct excitation/ionization or a K 1*s* excitation/ionization with subsequent X-ray emission causing a 300 as time delay. This delay has a dramatic influence on the recapture process.

Post-collision interaction (PCI) describes the interaction of a photoelectron and an Auger electron in the field of an ion. It is a manifestation of the fundamental three-body Coulomb problem and studied extensively for shallow core levels where the Auger decay occurs directly after ionization. Recent developments at light sources allow to study the PCI effect in new scenarios like cascade Auger decay or two-photon double ionization creating two photoelectrons.

Understanding the interaction between metal ions and their aqueous environment is of fundamental interest. We investigate Ca^{2+}(aq) ions at the 1*s* threshold using various hard X-ray techniques and quantum chemical calculations. In addition to normal Auger decay, ultrafast charge transfers from water to the calcium ion are observed, underscoring the complexity of the metal-solvent interactions. These findings provide deeper insights into the electronic properties of hydrated metal ions.

Application I Electronic Structure Friday, 17th April, 11:10

X-ray Standing Wave Imaging: Structure Determination of 2D Materials with Hard X-rays

Niclas Tilgner[1], Susanne Wolff[1], Serguei Soubatch[2], Tien-Lin Lee[3], F. Stefan Tautz[2], Thomas Seyller[1], Philip Schädlich[1], Christian Kumpf[2]

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Normal incidence X-ray standing wave (NIXSW) is a model-free approach for crystallographic structure determination with elemental specificity. The technique exploits the interference between incident and Bragg-reflected X-ray beams, which generates a standing wave field inside the bulk and at the surface of the crystalline substrate. By measuring the photoelectron yield of the atomic species, their positions relative to the standing wave – and thus with respect to the substrate lattice planes – can be determined. In essence, a single measurement captures both the amplitude and phase of the complex scattering factor for the selected Bragg reflection. By compiling a sufficiently complete set of such measurements using different reflections, the three-dimensional atomic distribution of species within the bulk and on the surface can be reconstructed (“imaged”) by a Fourier back-transformation.

Here, we employ NIXSW imaging to resolve the structural mechanism governing the formation of the quantum spin Hall insulator bismuthene at the interface between graphene and 4H-SiC. After Bi intercalation beneath epitaxial graphene and subsequent annealing, the ($\sqrt{3}\times\sqrt{3}$) reconstructed Bi β phase forms. Our measurements reveal that Bi atoms initially occupy the triply coordinated T_4 adsorption site, a configuration that prohibits the formation of bismuthene. Upon hydrogenation, however, one-third of the substrate bonds become saturated by hydrogen, allowing the Bi atoms to relax into T_1 top positions. This structural transition, unambiguously resolved by our NIXSW imaging experiment, enables interlayer σ-bonding and stabilises the two-dimensional Bi honeycomb lattice, thereby giving rise to the characteristic band structure of the quantum spin Hall phase.

Application I Electronic Structure **Friday, 17th April, 11:25**

Structure and Electronic Properties of Epitaxial Ultrathin Ni-Fe Oxide Films on MgO (001)

Jari Rodewald, Jannis Thien, Kevin Ruwisch, Tobias Pohlmann, Joachim Wollschläger

University of Osnabrück, Osnabrück, Germany

Ultrathin Ni-Fe oxide films are deposited on MgO (001) substrates at 250°C via reactive molecular beam epitaxy. Their Ni-to-Fe content was varied from 0 to 2. Near-surface composition and structure are studied by in situ soft-XPS and LEED. Detailed HAXPES studies of both Ni 2*p* and Fe 2*p* photoelectrons were performed to study the composition related electronic properties. Formation of Ni ferrite films ($Ni_xFe_{3-x}O_4$) is observed for low Ni content (x<1). Ni 2*p* shows the spectrum typical for Ni^{2+} content of Ni ferrite. Fe 2*p* points to coexistence of both Fe^{2+} and Fe^{3+} for small x while pure Fe^{3+} content is observed for stoichiometric Ni ferrite ($Ni_xFe_{3-x}O_4$, x»1). Only Fe^{3+} is also observed for x>1 while the Co 2*p* spectra point to formation of NiO as demonstrated by evolution of low binding energy shoulder of Ni $2p_{3/2}$. Thus, the Ni ferrite film is Ni saturated for x»1 ($NiFe_2O_4$). If the Ni content is increased beyond this value NiO precipitates are formed. AR-HAXPES demonstrates that both Ni and Fe are distributed homogeneously in the entire oxide films for all compositions. Thus, NiO precipitates are homogenously distributed in the stoichiometric

$NiFe_2O_4$ film. Complementary XAS experiments show that Fe^{2+} cations located on octahedral lattice sites are substituted by Ni^{2+} for the ferrite phase. Ni^{2+} cations are also on octahedral lattice sites for NiO precipitates. Varying the film thickness of $NiFe_2O_4$ films from 3nm to 60nm, no formation of NiO precipitates is observed but strong tetragonal distortion for films thinner than 15nm.

Application I Electronic Structure Friday, 17th April, 11:40

Lab-Scale HAXPES for Critical Buried Interfaces in III-V Heterostructures

Eugenie Martinez[1], Guy-Vano Tsamo Tagougue[1,2], Marc Veillerot[1], Vincent Thoréton[1], Mickael Martin[2], Thierry Baron[2], Franck Bassani[2]

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The recent development of instruments equipped with hard X-ray sources opens new perspectives for the use of HAXPES at the laboratory scale. It is an interesting technique for the non-destructive analysis of buried interfaces, offering new opportunities (1).

When combined with ion sputtering (Ar^+), this technique allows probing deeper than the damaged surface, minimizing the impact of sputter-induced artefacts. We illustrate this point with the study of III-V heterostructures, such as the InGaAs/InP/InAlAs/InP multilayer developed for radio-frequency applications. HAXPES is used to study the abruptness of the top InGaAs/InP interface, looking for possible elements interdiffusion (2). Modelling intensity ratios enable a precise estimation of the InGaAs residual thickness after sputtering, as well as the quantification of the InGaAs and InP compositions.

Laboratory tools also offer the possibility to combine lab-scale HAXPES with standard XPS using hard (CrKα) and soft (AlKα) X-ray sources. This approach enabled the investigation of Sb segregation in InP/GaAsSb/InP heterostructures. The depth-dependent composition was obtained through angular-dependent measurements. Modelling HAXPES intensity ratios at various angles provided evidence of Sb segregation in the top InP layer, as confirmed by grazing XPS measurements.

(1) O. Renault et al., *Faraday Discussions* **236**, 288 (2022).
(2) G. Tsamo Tagougue et al., *J. Appl. Phys.* **138**, 025301 (2025).

This work, carried out on the Platform for Nanocharacterisation (PFNC), was supported by the LabEx MicroElectronics (ANR-15-IDEX-02), by the "Recherche Technologique de Base" and the "France 2030 - ANR-22-PEEL-0014" programs of the French National Research Agency.

Application I Electronic Structure **Friday, 17th April, 11:55**

The Origin of the Fermi Level Pinning for Hf-Based Gate Stack Structures Studied by Operando Hard X-ray Photoelectron Spectroscopy

Yoshiyuki YAMASHITA

National Institute for Materials Science, Tsukuba, Japan. Kyushu University, Fukuoka, Japan

The remarkable downsizing of Si devices has led to a notable reduction in the gate dielectric film thickness, forming advanced gate all around (GAA) and CFET structures where the device structures are extremely small. One of the issues for such devices is the Fermi level pinning where the bias voltage is not applied correctly. In the present study, bias-dependent potential distribution in the advanced Si device structures was investigated to clarify the origin of the Fermi level pinning using operando hard x-ray photoelectron spectroscopy (OP-HAXPES).

Three kinds of Hf-based gate stack structure were prepared; Pt/HfO_2/SiO_2/Si(100), Pt/$HfSiO_2$/SiO_2/Si(100), and Ru/HfO_2/SiO_2/Si(100) structures. The OP-HAXPES measurements were performed at SPring-8 BL15XU. The incident photon energy was 5.95 keV while the total energy resolution was set to 240 meV.

Analysis of the core level peal positions as a function of the bias voltage indicated that a potential drop occurred at the Pt/HfO_2 interface for the Pt/HfO_2 gate structure while a potential gradient was not observed at the Pt/$HfSiO_2$ and Ru/HfO_2 interface for the Pt/$HfSiO_2$ and the Ru/HfO_2 gate structures. Angle resolved photoelectron spectroscopy revealed that a SiO_2 layer was formed at the Pt/HfO_2 interface, indicating that the origin of potential drop at Pt/HfO_2 interface is formation of the SiO_2 layer. Therefore, the Fermi level pinning might be attributed to the formation of the SiO_2 layer at the metal/high-k interface for metal/high-k gate stack structures.

Method Poster 1

The Challenge of Quantifying Photoemission Spectra Using Multiple Photon Energies

Thierry Conard[1], Anja Vanleenhove[1], Ilse Hoflijk[2]

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The development of Photoemission spectroscopy in laboratories during the last decades has been focused on the use of AlKα radiation (1484.6 eV). Extensive work has been performed to tackle the issue of quantification of acquired spectra. These include aspect such as the determination of sensitivity factor, understanding spectral background, determining transmission function of spectrometers, understanding electron transport inside materials (inelastic mean free path, …).

The use of higher energy photons (HAXPES) has the potential to significantly increase the application field of PES due to its larger depth information making it more suitable for multilayers systems. One of the major limitations of HAXPES is the strong decrease of the photoemission cross-section at higher photon energy which, until a few years ago limited the use of HAXPES to synchrotron, where higher photon flux are achieved than in laboratory instruments. As such, the challenges to quantify HAXPES spectra do not differ significantly from lower photon energy experiment, but this was not the prime focus of synchrotron-based experiment. With the introduction of performant laboratory-HAXPES systems a few years ago, the need of better quantification for HAXPES has strongly been increasing.

Next to the "classical" challenges, some additional aspects need (more often) to be considered. First, energy referencing is critical when chemical state quantification is required. Second, thanks to the larger photon energy, for many elements, additional photoemission peaks are available for analysis, and peak-independent quantification would be interesting. For both aspects, we will present examples of applications and improvements.

Method Poster 2

Advancements on the VerSoX Beamline B07 at Diamond Light Source: Expanding Capabilities for Near-Surface X-ray Spectroscopies

Pilar Ferrer, Matthijs A van Spronsen, Burcu Karagoz, David C Grinter, Santosh Kumar, Federica Venturini, Georg Held

Diamond Light Source, Didcot, United Kingdom

Versatile Soft X-ray (VerSoX) beamline B07 at Diamond Light Source facilitates studies of the surface chemical composition, electronic and geometric structure under different sample environments by X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy.

B07 consists of two branchlines, B and C, from a bending magnet source. The photon-energy range covers 170-2800 eV in C branch, and 45-2200 eV in B. The near ambient-pressure (NAP-XPS) endstation in C branch enables experiments at pressures up to 50 mbar, with capabilities for sample biasing and temperature variation (250–750 K at AP). B branch has two end stations: ES-1 provides a UHV system for XPS and NEXAFS (TEY, AEY, TFY, PFY) measurements, equipped with a standard sample preparation chamber (temperature range 120-1250 K); ES-2 supports NEXAFS under ambient conditions (10^{-7} mbar to 1 bar). Both branches accommodate specialised environments, including microreactors for heterogeneous catalysis, liquid and operando electrochemical cells.

As part of the Diamond-II upgrade, C branch will be replaced by a new NAP-XPS beamline with an undulator source covering the energy range 170 - 4000 eV. The monochromatisation of the X-rays will be achieved using a PGM with Cr/C multilayer (ML) grating for enhancing efficiency at higher energies. Preliminary tests under intense X-ray exposure and oxygen partial pressures of $\sim 10^{-8}$ mbar (Scientific Reports, 15, 35698, 2025) show resistance to corrosion/beam damage (verified through X-ray reflectivity, XPS and NEXAFS) and the expected improvement in resolution and flux in the range 1500-2800 eV.

Method Poster 3

EMIL Beamline: a "Two-Color" Spectroscopy Beamline Dedicated to Energy Materials at BESSY II

Mihaela Gorgoi[1,2], Xuchun Wang[1,2], Eva Lott[1,2], Raul Garcia-Diez[1], Michael Hävecker[2,3,4], Stefan Hendel[5], Simone Raoux[2,6], Will Smith[5], Markus Weigand[2,6], Regan Wilks[1,2], Jens Viefhaus[5], Marcus Bär[1,2,7,8]

[1]Interface Design, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Berlin, Germany. [2]Energy Materials In-situ Laboratory Berlin (EMIL), HZB, Berlin, Germany. [3]Fritz-Haber-Institut, Max Planck Society, Berlin, Germany. [4]Max-Planck-Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany. [5]Optics and Beamlines, HZB, Berlin, Germany. [6]Nanospectroscopy, HZB, Berlin, Germany. [7]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN), Berlin, Germany. [8]Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

EMIL is a joint state-of-the-art research infrastructure established by HZB, Fritz-Haber Institute (Max-Planck Society) and Max Planck Institute for Chemical Energy Conversion. It is dedicated to investigating energy materials by combining large-scale thin-film fabrication with advanced synchrotron-based spectroscopies. The platform specializes in comprehensive surface and interface analysis offering PES, HAXPES, XAS, XES, RIXS, XRF, and STXM that fully exploit the 80 eV to 10 keV energy range of the "two-color" EMIL beamline. The energy tunability and high resolution allow systematic control of information depth from Ångströms to micrometers, capturing chemical, electronic and structural properties.

In this contribution we will concentrate on the "two-color" EMIL beamline, a unique instrument that integrates two sources for soft and hard X-rays. The soft X-ray UE48 and hard X-ray in-vacuum cryogenic U17 undulators provide high brilliance and photon flux over a continuous energy range spanning 80 eV to 10 keV. The optical layout is designed to focus both branches at the same point in the three end-stations SISSY-I, OÆSE@SISSY-II, and CAT. Two other soft and hard X-rays foci serve MYSTIIC and PINK end-stations, respectively. The branches can be operated alternatively or simultaneously supplying X-rays to either the same or separate analytics systems.

Here we will present a comprehensive update on the status and performance of both EMIL branches. Key performance indicators - energy resolution, photon flux, and focus size, are reported. Furthermore, recent progress and technical challenges associated with the implementation of automated user operation will be discussed, together with planned optimization strategies and prospective upgrades.

Method Poster 4

In-situ Multimodal Study of PEG-Capped Au Nanoparticles using Standing-Wave Photoemission and Grazing-Incidence X-ray Scattering

Dongwoo Kim[1], Kyungmin Kim[2], Bongjin Mun[2], Slavomir Nemsak[3]

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Near-total reflection geometry in X-ray experiments enables tunable penetration depth and the formation of X-ray standing waves, providing a powerful approach for depth-resolved spectroscopy of complex interfaces. Here, we investigate the oxidation behavior of polyethylene glycol (PEG)-capped Au nanoparticles supported on a p-doped Si substrate using an in-situ multimodal approach combining standing-wave ambient pressure photoelectron spectroscopy (SWAPPS) and grazing-incidence X-ray scattering (GIXS). The SWAPPS results reveal that the PEG capping layer decomposes under O_2 exposure due to radical oxidizers generated by X-ray-induced dissociation of O_2 molecules. Concurrent GIXS measurements capture the corresponding structural evolution of the nanoparticle layer, indicating a displacement of the Au nanoparticles toward the substrate by ~2 nm following removal of the organic capping layer. Quantitative modeling of the X-ray optical field and photoemission signals using PyXRO enables reconstruction of the nanoparticle–substrate geometry with sub-nanometer accuracy. These results demonstrate the strength of a multimodal standing-wave approach combining photoemission and X-ray scattering to simultaneously resolve chemical and structural evolution at heterogeneous interfaces under realistic reaction conditions.

Method Poster 5

Lithographie on $SrCoO_x$ Thin Films for Hard X-Ray Momentum Microscopy at Beamline P22

Volkmar Koller[1], Sourav Chowdhury[2], Bojan Bosnjak[3], Rajan Mishra[4], Hans-Joachim Elmers[5], Olena Fedchenko[6], Sergii Chernov[1], Andrei Hloskovsky[1], Christoph Schlueter[1]

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Germany. [6]Goethe Universität Frankfurt, Frankfurtm am Main, Germany

Emerging memory devices could reduce electricity expenditure in the future compared to established complementary metal-oxide-semiconductors (CMOS). For instance, the Mottronic is based on a topotactic phase transition (TPT) associated with a metal-insulator transition (MIT) rather than charge manipulation, as it occurs in semiconductors. This could enable further miniaturization of devices.

Here, we show the Hard X-Ray Momentum Microscope (HarMoMic) at the beamline P22 of the PETRA III synchrotron at DESY as a tool to monitor the electronic and crystalline structure of materials exhibiting a TPT. Using Hard X-ray Photoelectron Spectroscopy (HAXPES) the HarMoMic probes the angle resolved bulk electronic structure of single crystalline samples. Thus, the electronic band structure and X-ray photoelectron diffraction patterns (XPD) can be measured. The crystalline structure of a material can be determined by comparing the XPD patterns to simulations (Kikuchi Diffraction patterns).

As a model system, we present measurements of $SrCoO_x$(001) thin films grown via PLD on Nb-doped $SrTiO_3$(001). When an electric bias is applied, the material undergoes a TPT, electrochemically oxidizing from $SrCoO_{2.5}$ (Brownmillerite, insulator, antiferromagnetic) to $SrCoO_{3-\Gamma}$ (Perovskite-like, metallic, ferromagnetic) undergoing a TPT.

Here, we depict our experience with lithographie for contacting and initial results upon biasing.

Method Poster 6

TPS - 47A2 High-Resolution HAXPES: Overview and Applications

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The TPS 47A2 HAXPES endstation is equipped with a SPECS PHOIBOS 150 NAP analyzer and a two-dimensional CMOS detector with true pulse counting, enabling high energy resolution and low-noise performance for probing buried interfaces and subsurface electronic structures. The system supports both synchrotron radiation and Al Kα / Cr Kα laboratory X-ray sources, allowing flexible operation from conventional XPS to HAXPES and multiscale analysis from surface to bulk. With a modular design, in situ biasing capability, and a wide temperature range of 15–1000 K, it provides a versatile platform for advanced HAXPES studies.

The endstation will be further integrated with the TPS-47A high-resolution beamline via a four-bounce high-resolution monochromator (HRM), delivering a narrow-bandwidth hard X-ray beam with sub-eV energy stability. This enables high-resolution HAXPES in the 3.5–10 keV range, combining deep probing depth, low noise, and high spectral resolution.

The platform focuses on operando and field-effect-controlled studies of semiconductor heterostructures, two-dimensional materials, and high-k dielectric interfaces, and will continue to incorporate diverse in situ and device-relevant environments to support next-generation semiconductor and functional materials research.

Method **Poster 7**

3D Mapping of Photoelectron Diffraction Patterns at Low Energies

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Photoelectron diffraction (PED) is a powerful method for determining the structure of materials, dopant sites, adsorbates and defects. In this study, we introduce a new 3D recording technique designed to maximize the amount of information obtained from the PED process. We studied the model systems Si (111) and Ge (111) at extremely low kinetic energies, close to the minimum of the inelastic mean free path (1). Measurements were performed using the combined hemispherical and time-of-flight momentum microscope (2) at beamline I09 at the Diamond Light Source. This instrument has a novel multimode front lens (3). Results were obtained for Si 2*p*, Si 2*s*, Ge 3*d* and Ge 3*p* core-level photoelectrons at kinetic energies between 35 and 400 eV. A full-field PED pattern with a diameter of ~8 $Å^{-1}$ is typically acquired in 5-10 minutes. The photon energy was varied in small steps of down to 2 eV. The circular dichroism contrast exhibits a rich fine structure and shows the well-known antisymmetry with respect to the mirror plane (4).

Even for identical kinetic energies, the PED patterns for Ge 3*d* and 3*p*, and Si 2*s* and 2*p* show significant differences. This emphasizes the importance of the orbital structure of the initial state. Theoretical calculations using the one-step photoemission approach (5) show good agreement with the measurements.

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Theory Poster 8

From Low- to High-Energy Photoelectron Diffraction: Novel Theoretical Approaches and Kikuchi Diffraction Analysis

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Time-of-flight based momentum microscopy (ToF-MM) is rapidly gaining traction in photoemission research. It enables simultaneous energy- and momentum-resolved acquisition of the full photoelectron distribution without sample tilting. The pronounced energy dependence of Kikuchi patterns (1,2) revealed by ToF-MM complicates their interpretation, necessitating advanced theoretical approaches. Recent advances in large k-field detection expand the accessible photon-energy range from 120 to 6000 eV. To address complex scattering mechanisms across this range and to distinguish these PED effects from angle-resolved photoemission spectroscopy (ARPES), we present a theoretical study of fine diffraction patterns and their energy evolution.
We simulate core-level emissions from Ge (100) and Si (100) using multiple-scattering theory and the fully relativistic one-step photoemission model (3). Faint diffraction networks are reproduced for various core levels over kinetic energies from 35 eV to 4174 eV, avoiding cluster-size convergence limitations inherent to cluster-based approaches. Pattern broadening is analyzed via inelastic scattering. For the first time, we reproduce circular dichroism in the angular distribution of Si (100) 1s photoelectrons, revealing asymmetries up to 31% (4). We further investigate PED at very low kinetic energies relative to the inelastic mean free path near the minimum of the universal curve. The results show remarkable agreement with experimental data obtained using circularly polarized radiation.

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Application I Electronic Structure **Poster 9**

Investigation into the Effects of Structure on Gallium Oxide using X-ray Photoelectron Spectroscopy

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β-Ga_2O_3 is an ultra-wide band gap semiconductor (E_g ~ 4.8 eV) with a large Baliga figure of merit, making it an emerging material for power electronics. (1) Whilst its bulk electronic structure is well established, its facet-dependent variations remain relatively unresolved, despite their relevance in device interfaces.

Here, hard X-ray photoelectron spectroscopy (HAXPES) at beamline I09 (Diamond Light Source) is used to probe the bulk-sensitive electronic structure of β-Ga_2O_3 single crystals on exposed (100), (010), (001) facets. (2) The increased probing depth at higher photon energies enables distinction between bulk and surface contributions to core, semi-core, and valence spectra. (3) Comparison with soft X-ray PES allows determination of intrinsic and extrinsic features, enabling quantification of surface-dependent spectral changes. Experimental results are interpreted alongside first principles calculations to resolve facet and orbital dependent electronic variations.

These results highlight the utility of HAXPES to disentangle complex bulk and surface electronic structure and to resolve facet-dependent electronic variations important to device performance.

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Application I Electronic Structure **Poster 10**

A Complementary in-depth Analysis of Composition and Band Bending at the Topological Insulator and Superconductor Interface using Lab-Based HAXPES and XPS

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One avenue towards building a topological qubit for quantum computing involves creating and manipulating Majorana zero modes in a hybrid device comprising s-wave superconductors and 3D topological insulators (TIs). For this purpose, the Fermi energy ideally lies at or close to the Dirac point. The Fermi level within a BiSbTe (BST) can be precisely tuned by adjusting the Bi:Sb stoichiometry in the TI and can be mapped via ARXPS (1). However, once the required superconducting material is deposited on top of the TI, the Fermi level shifts depending on the work function of the material in contact. Stack layouts and thickness could make it inaccessible with conventional XPS, hence HAXPES is required.

A complementary study of lab-based HAXPES and XPS under UHV on TIs with superconductor interfaces is minimal in literature. This study focuses on the interfacial behavior of BST with superconductors, with a focus on Pt and on Nb. Both Ar ion sputtering and angular resolved analysis using hard (CrKΓ) and soft (AlKα) X-rays help track the change of composition throughout the stacks and interfacial band bending.

The band bending at the interface can be experimentally modeled using angle resolved analysis based on HAXPES and XPS. The information depth is dependent on the IMFP of the materials. The energy shift depth profile for Bi $4f_{7/2}$, Sb $3d_{5/2}$ and Te $3d_{5/2}$ reveals n- or p-type behavior at the interface to the superconductors.

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Application I Electronic Structure **Poster 11**

Emergent Hybrid Quasi-Modes in Magnetic Weyl Semimetal NdAlSi

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Magnetic Weyl semimetals have emerged as a fertile ground for exploring new quantum phases of matter and quasiparticles. The latter includes unconventional fermions with larger Chern numbers than those of conventional Weyl fermions and topologically non-trivial band structures in bosonic excitations. In this direction, our theoretical findings predict the presence of chiral phonons with non-zero pseudo angular momentum in NdAlSi. Furthermore, in the field-induced ferromagnetic phase, we observed a huge increase in magneto-thermal conductivities that was related to the topological magnon-polaron, emerging from the hybridization of the chiral acoustic phonons with the magnons. These topological excitations carry heat in the presence of a magnetic field, suggesting an important role for chiral phonons in heat transport, such that the conductivity is substantially modulated by a magnetic field. However, gaining direct insight into these quasi modes remains a significant challenge, underscoring the complexity of the research. This complexity underscores the crucial role of inelastic scattering spectroscopic techniques using X-rays.

Application I Electronic Structure **Poster 12**

Electronic Structure of Sn-doped In_2O_3 Films Investigated by Hard and Soft X-ray Photoelectron Spectroscopy

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Post-annealing is widely employed to tune the electrical performance of Sn-doped In_2O_3 (ITO) by modifying defect chemistry and carrier density under oxidizing and reducing environments. In particular, O_2 and H_2 annealing provide an effective route to control oxygen vacancies and donor states, thereby significantly influencing the transport properties of ITO films. However, despite its technological importance, the depth-dependent evolution of the electronic structure induced by gas annealing remains insufficiently understood, especially regarding the distinct responses of the surface and bulk regions.

In this work, we systematically investigate the depth-dependent electronic structure of ITO films annealed under O_2 and forming gas (Ar 96% + H_2 4%) using complementary soft X-ray photoelectron spectroscopy (XPS) and hard X-ray photoelectron spectroscopy (HAXPES). HAXPES measurements reveal that the bulk stoichiometry remains nearly unchanged regardless of annealing ambient, whereas XPS indicates an In-rich and oxygen-deficient near-surface region after annealing. Valence band analysis further shows that the valence band maximum (VBM) increases with annealing temperature under forming gas, while it decreases under O_2. Notably, the VBM values obtained from XPS are systematically larger than those from HAXPES for all annealing conditions. This persistent offset indicates pronounced surface–bulk electronic decoupling in ITO films, which is attributed to surface-related band bending and/or electron accumulation effects that are relatively insensitive to the annealing ambient. These findings highlight the importance of depth-resolved photoemission for correctly interpreting the electronic structure of transparent conducting oxides.

Application I Electronic Structure **Poster 13**

Circularly Polarized Resonant Study of the Electronic Band Structure in an Oxide Dice-Lattice

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Flat-band materials have attracted intense interest since they provide a platform where electronic interaction can overwhelm kinetic energy, potentially exhibiting unconventional magnetism, superconductivity, and topological phases. The dice lattice is a prototypical geometry hosting a dispersionless flat-band intersecting Dirac cones. Recent theoretical study predicts that a (111)-oriented $LaMnO_3/LaAlO_3$ (LMO/LAO) dice lattice can realize an electronic structure with a nearly flat-band at the Fermi level, potentially stabilizing ferromagnetic order. Here, we investigate a (111) oriented LMO(3uc)/LAO(4uc) superlattice film. Magnetization measurements reveal an antiferromagnetic transition at $T_N \sim 17$ K with a magnetic moment of ~2 μ_B per Mn. In contrast, a reference LMO (111) film shows canted antiferromagnetism with $T_N \sim 75$ K with clear M-H hysteresis at low temperature. Resonant photoemission near the Mn *L*-edge enhances Mn-derived states

just below the Fermi level. Circular dichroism in the density of states (CD-DOS) emerges below 100 K and increases upon cooling to lowest accessible temperature of 30 K, consistent with the magnetization measurement. Resonant ARPES unexpectedly reveals spin-split band dispersions within 1 eV below the Fermi level. Although neither a flat band at the Fermi level nor ferromagnetic instability is observed, the overall dispersion is in good agreement with the calculated antiferromagnetic band structure. However, due to interfacial symmetry breaking in the dice lattice, the observed spin splitting may be affected by Rashba-type spin orbit coupling alike.

Application I Electronic Structure **Poster 14**

Study of Buried Interface of Transition Metal Oxides with Multimodal X-ray Analysis

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In complex oxides, "intertwined" charge, spin, orbital, and lattice degrees of freedom are a central organizing concept: their strong mutual coupling generates many of the exotic phases and functionalities pursued in quantum-materials research. Specially, at buried oxide heterointerfaces, the breakdown of interfacial symmetry and the mutual reconfiguration of these charge, spin, orbital, and lattice degrees of freedom give rise to entirely new quantum states that do not exist in the bulk.

Using various tender X-ray–based spectroscopies—such as tender X-ray grazing-incidence ambient-pressure photoelectron spectroscopy, grazing-incidence X-ray scattering, and X-ray diffraction at DESY-Petra III, Germany and PLS-II, Korea, we explored the physical and chemical properties of buried interfaces as a topotactic phase transition, an ion-migration-driven structural phase transition, takes places on heterostructures of transition metal oxides system, e.g., LaMnO3 on SrTiO3 substrate. During the topotactic phase transition, the structure and chemical states of interfacial layers show clear modification, indicating its strong involvement in the phase transition. The correlation between interfacial structures and its topotactic phase transition will be discussed.

Application I Electronic Structure Poster 15

Probing Buried Interfaces Under Bias: Operando HAXPES on Advanced Ferroelectric Devices

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Ferroelectric hafnium zirconium oxide (HZO) films are highly attractive for non-volatile memory in neuromorphic computing, offering significant reductions in AI power consumption alongside straightforward compatibility with Si-based processing and industrial scalability. Their operation relies on switching a remanent electrical polarization by an applied field; however, the atomistic mechanisms at the buried oxide–semiconductor interface during repeated cycling remain poorly understood. Probing these interfaces requires operando measurements on fully processed devices: conventional XPS lacks the probing depth to reach buried layers non-destructively, making HAXPES essential.

Operando HAXPES enables direct access to buried interfaces in functional devices under realistic operating conditions, revealing the interplay between electrical operation and chemical interface structure. Here, we demonstrate measurements on fully processed, wire-bonded InAs–$Hf_xZr_{1-x}O_2$–TiN metal–oxide–semiconductor devices tailored for operando HAXPES.

Measurements were performed at photon energies of 3–9 keV providing depth-resolved chemical sensitivity from the metallic top electrode to the buried semiconductor interface. Advanced electrical pulsing sequences, including Positive-Up Negative-Down (PUND) protocols, were implemented directly at the Galaxies beamline (synchrotron Soleil), enabling correlation of polarization switching with simultaneous chemical-state evolution.

Operando HAXPES reveals unexpected interfacial behavior during repeated switching: while electrical measurements confirm ferroelectric domain reversal, depth-sensitive core-level spectra indicate progressive redox reactions at the buried InAs–oxide interface. This demonstrates that device operation induces interfacial modifications inaccessible by ex situ analysis.

Our results demonstrate the capability of modern HAXPES beamlines to study realistic device architectures under functional conditions, opening new avenues for investigating switching dynamics, fatigue, and interface chemistry.

Application I Electronic Structure **Poster 16**

Hard X-ray Photoemission Study of Possible Thermoelectric Al-Pd-Ru Quasicrystals: Effects of Annealing and Si-Doping

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Al-based quasicrystals (QCs) are expected to exhibit high thermoelectric performance due to their deep pseudogap structure near the Fermi level (E_F) and complex crystal structures (1). However, to utilize Al-based QCs as thermoelectric materials, it is necessary to improve the Seebeck coefficient S. It has been reported that S of the Al-Pd-Ru QC is improved by annealing or Si-doping (2). Since S depends on the density of states (DOS) near E_F, the microscopic electronic structure should be experimentally examined. Previously, we have performed hard X-ray photoemission spectroscopy (HAXPES) and X-ray absorption spectroscopy of the non-annealed Al-Pd-Ru QC for revealing the electronic structure (3,4). We have also investigated the annealing and doping dependence of HAXPES spectra of the Al-Pd-Ru QCs.

The HAXPES experiments were performed at BL09XU in SPring-8 (5). The Al 2*s*, Ru 3*d*, and Pd 3*d* core-level peaks of the annealed and Si-doped Al-Pd-Ru QC all shift toward the lower binding energy side compared to those of the non-annealed Al-Pd-Ru QC, which suggests a rigid-band-like shift corresponding to the hole doping. The increase in the DOS at E_F due to the E_F shifting away from the bottom of the pseudogap structure would be responsible for the improvement of S.

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Application I Electronic Structure Poster 17

Momentum-Resolved Electronic Structure of $SrNbO_3$ Thin Films

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The realization of quantum materials (QMs) with both electron correlations and topological properties is currently under active investigation. In this context, 4*d* transition metal oxides offer a good balance between e-e correlations and spin-orbit coupling. Recently, a topological band structure was predicted for tetragonal $SrNbO_3$ (SNO) (1), featuring high mobility and linear magnetoresistance (2,3). The understanding of its band structure is still not well established experimentally. In fact, the synthesis of pristine SNO thin films is challenging due to the metastable nature of the Nb^{4+} cation with a d^1 configuration. Here, we probe the 3D band structure of stoichimetric SNO thin films on $DyScO_3(110)$ using photon energy and polarization-dependent soft X-ray photoelectron spectroscopy with the momentum microscope of beamline I09 at Diamond Light Source, UK. While the Fermi surface contours and band dispersions show overall good agreement with density-functional theory calculations, waterfall-type spectral weight between 1-2.5 eV at the Γ points has no counterpart in theory. We discuss its nature in terms of e-e correlations and coupling to lattice degrees of freedom.

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Application I Electronic Structure Poster 18

Exploring Oxide Membranes by Hard X-ray Photoemission Spectroscopy

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Freestanding oxide membranes have recently emerged as a versatile

platform for the design and control of novel electronic phases, either in their intrinsic form or via the formation of interfaces with broken symmetries (1). In a heterostructure consisting of a $SrTiO_3$ (STO) membrane with fourfold symmetry and an Al_2O_3 (sapphire) substrate exhibiting threefold interfacial symmetry, electron energy-loss spectroscopy (EELS) in scanning transmission electron microscopy (STEM) revealed indications of charge transfer into the Ti 3*d* states of the STO membrane (2). The microscopic mechanism underlying this electron transfer, however, remains unresolved.

To gain further insight, we investigated the evolution of the Ti^{3+} spectral weight using hard X-ray photoelectron spectroscopy and compared the experimental results to theoretical simulations across a range of membrane thicknesses, down to the ultra-thin limit of 2 unit cells of STO.

Another membrane material in application is $LaTiO_3$, attracting significant interest due to its Mott insulating behaviour (3). We established the fabrication of membranes to integrate them into a strain device. This offers a promising route toward reversible control of the Mott transition and may pave the way for the active manipulation of correlated phase transitions in other freestanding oxide membrane systems by strain.

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Application II Energy Poster 19

Direct Observation of Hydrogen-Driven Surface Evolution of HEA Revealed by in situ XPS and NEXAFS from 1 mbar up to 1 bar

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The evolution of the surface electronic structure of High Entropy Alloy (HEA) was investigated using synchrotron-based X-ray Photoelectron Spectroscopy (XPS), Near-Ambient Pressure XPS (NAP-XPS), and Near-Edge X-ray Absorption Fine Structure (NEXAFS) under sequential activation conditions, involving high and moderate hydrogen pressures and various heating degrees. A reference sample was measured under Ultra High Vacuum (UHV) for comparison. The following samples were measured at moderate pressure in the NAP cell, high pressure in the HPR, and laser heating in the NAP. The findings show a selective reduction process on the HEA surface, where Fe is fully reduced to the metallic state. In contrast, Mn exhibits mixed oxidation states because of its multivalent nature, while Ti and Zr present a resistance toward a full reduction by maintaining their partial oxide and suboxide states. This combination created by the hydrogen-induced electronic restructuring, is useful for the hydrogen absorption and desorption process, as the metallic states are efficient for hydrogen dissociation; meanwhile, the suboxide state helps hydrogen diffuse inside the alloy.

Application II Energy **Poster 20**

Interphase Dynamics in Anode-Free Lithium Batteries Studied with Operando-HAXPES

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Anode-free lithium batteries employing solid polymer electrolytes (SPEs) offer significant promise for high-energy density storage but face critical challenges at the current collector interface, such as to copper, where interfacial reactions strongly influence stability. Using operando hard X-ray photoelectron spectroscopy (HAXPES), here employed both at the HIKE end-station at BESSY II and in our in-house HAXPES-lab, the interfaces between SPE and metal current collectors can be studied. Taking advantage of the chemical sensitivity of HAXPES and the different photon energies both the SPE and interface with the current collector can be studied showing processes such and lithium migration, interphase decomposition and oxidation processes under realistic conditions. Here we also address the thin current collectors needed to probe through to the SPE. This type of study underscore processes such as Li transport and interfacial redox processes and how they govern interfacial stability and highlight the need for interface engineering to optimize anode-free all-solid-state battery performance.

Application II Energy **Poster 21**

Controlling Jahn–Teller Distortion through Mn Slab Localization for Stable High-Voltage Sodium-Ion Batteries

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Mn-rich layered oxides are among the most promising cathode materials for large-scale sodium-ion batteries due to their high capacity, elemental abundance, and low cost. Nevertheless, the practical application of these materials is impeded by the pronounced and intractable Jahn–Teller effect associated with Mn^{3+} ions. This effect triggers cooperative lattice distortion, resulting in structural degradation and compromised cycling stability.

In this work, we demonstrate that spatially localizing Jahn–Teller active Mn^{3+} ions within confined Mn-rich slabs effectively suppresses long-range distortion and stabilizes the layered framework. The engineered Mn-rich oxide, $NaNi_{0.3}Cu_{0.1}Mn_{0.6}O_2$ (NCM316), exhibits exceptional electrochemical performance, achieving 89.5% voltage retention after 200 cycles. In full-cell configurations, NCM316 delivers a high discharge voltage of 3.36 V, the highest reported for Mn-based layered cathodes, while maintaining 84% capacity retention after 500 cycles and reaching an energy density of 337 Wh kg^{-1}, outperforming all other Mn-based layered cathodes under a high cutoff voltage of 4.4 V. Comprehensive characterization using synchrotron X-ray and neutron scattering techniques, supported by theoretical simulations, confirm the localized presence of Mn^{3+} and elucidate its role in maintaining structural integrity and mitigating adverse interactions with neighboring transition metals. This work offers insight into the mechanism of Jahn–Teller distortion in Mn-rich layered oxides and proposes a broadly applicable design principle for stabilizing other Jahn–Teller active systems, such as layered lithium-rich cathodes, spinel-type oxides, and manganese-based materials for aqueous batteries.

Application II Energy **Poster 22**

Combining Experimental Design and Software Based Image Recognition for Operando APXPS Electrode/Electrolyte Interface Potential Probing

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Probing the electrode/electrolyte interface with operando APXPS in the dip-and-pull setup remains fundamental challenges on 1) forming a stable interface, 2) probing through the liquid layer with limited XPS probing depth, and 3) probing at an electrochemically active interface. Apart from the fundamental challenges, experimental uncertainties on liquid variations over time, space, and irradiation effect amplify the difficulties on operando interface probing.

In this work, an efficient interface probing methodology is realized through experimental design combined with advanced data processing. Scanning APXPS is employed with programmed route periodically probing across the dry-wet boundary near the top edge of the liquid layer to capture the interface spectroscopic feature. To recognize and select the interface-featured spectra, software based spectroscopic recognition are developed including two methods 1) intensity attenuation recognition which distinguishes the interface-featured from the intensity attenuation of the electrode signals when scanning across the liquid layer 2) potential recognition which selects the interface-featured spectra by its BE shift over the height in the meniscus.

Further by translating the relative intensity of the electrode and electrolyte peaks into liquid thickness, a spectro-microscopic imaging of the liquid distribution with topographical resolution is obtained. Combining with the spectral energies and chemical distribution information, it sees strong correlation between the energetics and the liquid layer thickness of the probing position, which is suggested to do with the EDL potential drop in the probed region. In addition, the chemical change of the electrode (lithiation, etc) also highly affects the interface potential drop.

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Using Hard X-ray Photoelectron Spectroscopy to Probe the Impact of the Sulfur-To-Oxygen Ratio on the Chemical and Electronic Structure of Zn(O,S) Thin Films for Photovoltaic Applications

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Zn(O,S) is an n-type semiconductor that is commonly used in chalcopyrite- and perovskite-based thin-film solar cells, optoelectronic devices, chemical sensors, and thin-film transistors. The tunable optical band gap, which can be varied from 2.6 to 3.4 eV by changing the S/(S+O) (SSO) ratio, enables a tailoring of Zn(O,S) to specific device requirements. A systematic depth-resolved understanding of the impact of the SSO on the chemical and electronic structure, including the local chemical bonding and the band edges, is essential for further insight-driven optimization.

In this contribution, we employ hard x-ray photoelectron spectroscopy (HAXPES) and the X-SPEC beamline at the KIT Light Source, which enables depth-resolved measurements of both the chemical and electronic structure. We investigate sputter-deposited Zn(O,S) films relevant for Cu(In,Ga)Se_2 solar cells, with SSO ratios of 0, 20, 30, 40, 50, 60, 80, and 100 %. The HAXPES data is complemented by x-ray emission spectroscopy (XES) and optical bandgap measurements (UV-Vis).

We find significant variations of the chemical structure as a function of SSO, including the formation of sulfates, sulfites, and hydroxides at different depths of the films. With increasing SSO, the valence band shows a significant shift (> 1 eV) towards the Fermi energy. In our contribution, we will discuss our results and how they provide direct insights into the impact of the SSO on the chemical and electronic structure of Zn(O,S). We demonstrate the power of HAXPES to aid in the development of applied materials systems.

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Evaluation of Polymorphism and Charge Transport in a BaO–CaO–Ta2O5 Perovskite Phase Diagram using TOF-Neutron and Synchrotron X-ray Diffraction, the Bond-Valence Method and Impedance Spectroscopy

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Ba-based perovskite oxides exhibit excellent chemical stability and tunable electrical and catalytic properties through compositional modification. A representative example is $Ba_3Ca_{1.18}Nb_{1.82}O_{8.73}$, a ceramic proton conductor used in all-solid-state steam electrolysis and solid oxide fuel cells (SOFCs). Structural ordering in these materials strongly depends on composition and directly influences their functional properties. In this work, we establish a comprehensive phase diagram for the Ba–Ca–Ta–O quaternary perovskite system $Ba_3Ca_{1+x}Ta_{2-x}O_{9-3x/2}$ ($0 \leq x \leq 0.36$) over a wide temperature range (1000–1550 °C), complemented by theoretical calculations to probe cation ordering in supercells. The effect of cation clustering on O^{2-} diffusion pathways was also examined. Precise cation arrangements and structural characteristics were determined using time-of-flight neutron diffraction and synchrotron X-ray diffraction. The results reveal the potential of Ba–Ca–Ta–O compositions for functional applications.

Electrochemical properties were systematically analyzed using impedance spectroscopy genetic programming (ISGP). Electrical conductivity increases with x from 0 to 0.27, then decreases at $x = 0.36$ due to reduced mobile charge carrier concentration. In dry air, conductivity rises continuously across the entire composition range. In contrast, under humid conditions, only $Ba_3Ca_{1.18}Ta_{1.82}O_{8.73}$ (BCT18) and $Ba_3Ca_{1.27}Ta_{1.73}O_{8.595}$ (BCT27) show enhanced conductivity, indicating that cation clustering and defect chemistry are sensitive to oxygen partial pressure. These findings highlight the critical role of composition-controlled ordering and clustering in governing transport behavior in Ba-based perovskite oxides.

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Atomic-Scale Characterization of Spontaneously Formed Interfacial Layers at Metal/Polyimide Interfaces by HAXPES and STEM-EELS.

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Driven by the rapid spread of artificial intelligence technology, the semiconductor industry is experiencing unprecedented growth. Consequently, research in the field of semiconductor packaging—where the interface between metals and organic insulating materials, such as polyimide, determines device performance and long-term reliability—has become increasingly critical. As devices become increasingly highly integrated and miniaturized, understanding the chemical and structural properties of buried metal/organic material interfaces at the atomic level is an urgent scientific and technological challenge. In particular, the interface reaction layer spontaneously formed between metal and polyimide during the manufacturing process is known to significantly impact adhesion strength, thermal stability, and long-term durability. However, because this interface is buried, capturing its true nature non-destructively and with high spatial resolution is challenging, and its atomic-scale structure and chemical bonding state remain poorly understood.

Here, we developed analytical techniques to comprehensively elucidate the atomic-scale structure and chemical state of the spontaneously formed layer at the metal/polyimide interface (1). By complementarily combining hard X-ray photoelectron spectroscopy (HAXPES), performed at SPring-8 BL16XU, which enables non-destructive evaluation of the chemical state of buried interfaces, with scanning transmission electron microscopy–electron energy loss spectroscopy (STEM-EELS), which allows analysis of nanoscale structure and electronic states, we achieved quantitative evaluation of the composition, bonding state, and spatial distribution of the interfacial reaction layer. This presentation reports on the details of the established analytical method and its application results to the Ti/polyimide interface.

(1) Y. Kubo et al., *Appl. Surf. Sci.* 721, 165462 (2026).

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HAXPES of Buried Cu/Ethyl cyanoacrylate Interfaces.

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As efforts to achieve carbon neutrality gain momentum, reducing fuel consumption and CO_2 emissions in the automotive and aerospace sectors has become a challenge. With the adoption of lightweight composite structures using alloys and carbon fiber reinforced plastics, adhesive bonding technology is key to achieving joining of materials, surpassing welding methods. However, the mechanisms governing bond strength and durability at the interface between metal and adhesives remain understood. Specifically, the relationship between the chemical bonding at the interface, the formation of reaction layers, and adhesive performance is still unclear. As a result, adhesive development relies on empirical peel testing, making it difficult to predict and suppress degradation under real-world conditions (thermal cycling, humidity, fatigue). Epoxy structural adhesives are used in the transportation industry, but their interfacial chemistry is complex. This research adopts ethyl cyanoacrylate (ECA) as a model adhesive system to elucidate universal bonding principles on important metal surfaces.

Using a dedicated sample preparation method developed in-house (1,2), we positioned the Cu/ECA interface 50 nm below the Cu surface. We confirmed the sample structure via STEM-EELS and laboratory XPS. HAXPES using 8 keV photons at SPring-8 BL16XU (Proposal No. 2025R5030) yielded high-resolution C 1*s*, N 1*s*, and O 1*s* spectra, enabling sensitive detection of Cu-adhesive interactions (including Cu–N coordination and reaction layer formation). In the presentation, I will discuss the details of the interaction.

(1) Y. Kubo et al. *ACS Appl. Mater. Interfaces* 10, 44589 (2018).
(2) Y. Kubo et al. *ACS Appl. Nano Mater.* 5, 6757 (2022).

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