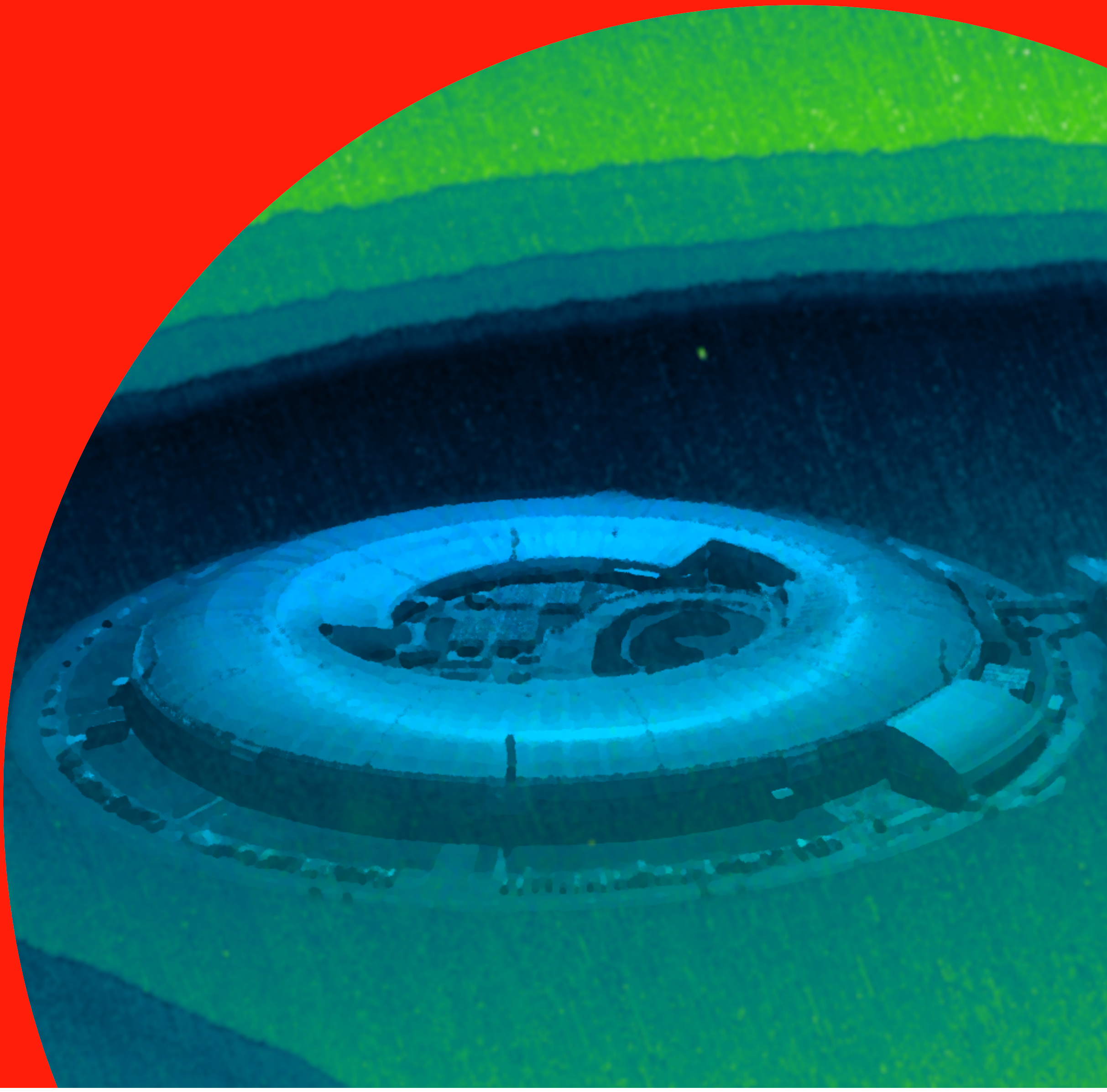
ISSC 2025

Interdisciplinary Surface Science Conference

31 March – 2 April 2025
Worcester College, Oxford, UK



iop.org

in partnership with Diamond Light Source

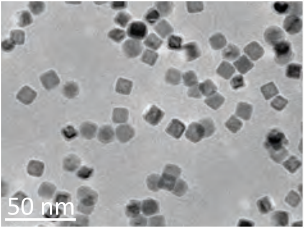
diamond

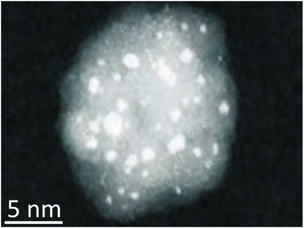
IOP Institute of Physics

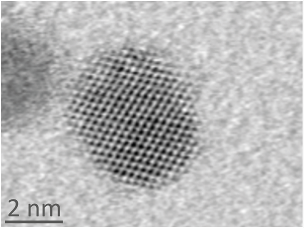
ISSC 2025

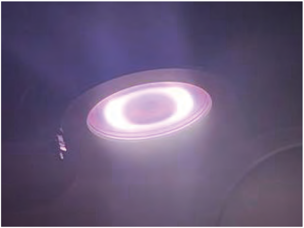
Page no.


nika LYTE
Nexus
nika LYTE
Nexus


50 nm


5 nm


2 nm



AEOLOS 150 & **ASTRAIOS** 190

THE NEXT GENERATION ELECTRON ANALYSERS
OPTIMISED FOR ARPES OR XPS, HAXPES AND NAP-XPS

AEOLOS 150

- Transmission-optimised design
- Parallel angle detection, over 60°
- Operation up to 10 keV
- Pulse counting AD-CMOS detector
- For XPS, HAXPES and NAP-XPS

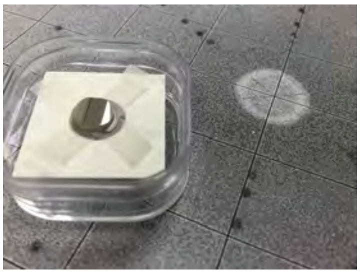
ASTRAIOS 190

- Single spot parallel shifting lens
- ± 30° acceptance angle
- Energy resolution <1.5 meV
- Motorised entrance slit
- For ARPES and Spin-ARPES

SPECS Surface Nano Analysis GmbH

VSM INSTRUMENTS **Our Business Partner in UK and Ireland**
VSM Instruments www.vsm-instruments.com

SPECS™
A member of SPECSGROUP



Does Morphology Drive CO_2 Reduction by Copper Oxide Catalysts? Insights from In Situ Analysis

Arrigo R[1]
[1]Salford University

Contributed speaker 23 - Rosa Arrigo, April 2, 2025, 10:40 - 11:00

S. Esmael Balaghi1,2, Michael Greenwood3, Heba Elgamodi3, Dhruv Trivedi4, Hamza Annath4, Diego Gianolio5, Manfred E. Schuster6, Marc G. Willinger7, Kathryn Toghill4, Rounack Kundu1, Zeljka Krpetic3, Anna Fischer1,2,8, Rosa Arrigo3,5
1Freiburg Center for Interactive Materials and Bioinspired Technologies (FIT), University of Freiburg, Germany;
2Freiburg Materials Research Center (FMF), University of Freiburg, Germany;
3School of Science, Engineering and Environ-ment, University of Salford, Manchester M5 4WT, UK;
4Department of Chemistry, Lancaster University, Lancaster, LA1 4YB, UK;
5Diamond Light Source Ltd., Harwell Science & Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK;
6John-son Matthey Technology Centre, Reading, RG4 9NH, UK;
7Department of Chemistry, Technical University of Munich, Lichtenbergstrasse 4 D-85748 Garching, Munich, Germany;
8Institute for Inorganic and Analytical Chemistry (IAAC), University of Freiburg, Germany.

Copper nanostructures-based electrocatalysts remain the best system for CO_2 electroreduction (CO_2RR) to energy-rich chemicals. In this study, we investigate a surfactant-free synthesis to produce monodisperse Cu_2O-based nanoparticles (NPs) with controlled morphology. We explore factors such as initial solution pH and dissolved gases in the reaction medium influencing nanoparticle morphology. An argon atmosphere enables a rapid and controlled synthesis of Cu_2O NPs, with shapes varying from round-edged cubes at neutral pH to a novel popcorn-like morphology (nanopopcorns, NPCs) at pH levels below 10, and sharp-edged cubes (nanocubes, NCs) above 10.5. In-situ X-ray absorption fine structure (XAFS) combined with UV-Vis spectroscopy during the formation of the Cu_2O nanoparticles suggests a complex mechanism of dissolution and condensation equilibria of Cu-hydroxide species at the particle/solution interface, with relative kinetics dictating particle shape and size. In-situ electrochemical liquid scanning transmission electron microscopy (EC-LSTEM) reveals that NPCs exhibit higher stability under CO_2RR conditions compared to NCs. CO_2RR tests show that NPCs achieve higher faradaic efficiencies for C–C coupling products at lower overpotentials, indicating improved performance over the commonly reported NCs, which increase ethylene production only at higher potentials and have a higher propensity for hydrogen evolution. This study sheds new light into the correlation between nanoparticle morphology and enhanced selectivity towards ethylene.

New Insights into CO Adsorption on TiO2(110): Enhanced IRAS characterisation

Barama N[1], Eder M[1], Sokolović I[1], Reticcioli M[2], Rath D[1], Schmid M[1], Diebold U[1], Pavelec J[1], Parkinson G[1]
[1]Institute of Applied Physics, TU Wien, [2]Faculty of Physics and Center for Computational Materials Science, Universität Wien

Contributed speaker 7 - Nail El Hocine Barama, March 31, 2025, 17:00 - 17:20

TiO_2(110) serves as a model system for investigating surface reactivity and catalytic behavior, with CO adsorption commonly employed as a probe molecule. While previous IR spectroscopy studies identified two distinct adsorption sites for low coverages (≤ 0.3 ML), regular Ti sites, and Ti sites near oxygen vacancies[12], recent work based on DFT and microscopy suggests the existence of additional adsorption configurations influenced by the polaronic nature of the substrate[3].
In this contribution, we present experimental results obtained using our custom-built reactivity and infrared reflection absorption spectroscopy (IRAS) setup[4]. This design, optimized for detecting small concentrations of adsorbates on metal oxide surfaces, delivers high-resolution spectra with a high signal-to-noise ratio, allowing us to observe new features. Our data reveal multiple CO adsorption configurations on TiO2(110), which agrees with STM observations from a recent study[3]. Additionally, these results demonstrate the potential of IRAS to guide and validate theoretical approaches.

References:

1. Xu, M. et al. Angew. Chem. Int. Ed. 51, 4731–4734 (2012).
2. Petrik, N. G. & Kimmel, G. A. J. Phys. Chem. Lett. 3, 3425–3430 (2012).
3. Reticcioli, M. et al. Phys. Rev. Lett. 122, 016805 (2019).
4. Rath, D. et al. Rev. Sci. Instrum. 95, 065106 (2024).

Surface degradation of NMC cathodes in contact with air

Bjorklund E[1], Weatherup R[1]
[1]University of Oxford

Contributed speaker 24 - Erik Bjorklund, April 2, 2025, 12:10 - 12:30

One of the most common cathode material in lithium-ion batteries is LixNi1-y-zMnyCozO2 (NMC), where the research is currently trying to increase the nickel content in order to increase its capacity. However, the high nickel content also makes the surface more reactive towards side reactions during electrochemical cycling leading to a shorter lifetime. It has also been found that as NMC is exposed to air it will also degrade the surface, further making the cycle life shorter. It has been suggested that curing the reaction with air the NMC can react with H2O to form a LiOH layer and that once the layer is thick enough further side reactions would be prevented. The passivation is assumed to be caused by deintercalation of lithium, where the thin disordered rock salt layer would mitigate the Li+-water reactions through decreasing the amount of lithium deintercalation.
In this study the surface interactions of NMC electrodes during air exposure will be presented using a combination of different techniques including ambient pressure XPS (NAP-XPS), soft x-ray absorption spectroscopy (XAS) and photoemission electron microscopy (PEEM). This will give understanding of how CO2 and H2O cause surface reduction and unideal surface layer formation affecting the electrochemistry.

Rotational orientation effects in hydrogen surface scattering

Chadwick H

Invited speaker 6 - Helen Chadwick, April 1, 2025, 11:20 - 11:50

Hydrogen is the most abundant molecule in the universe, and its interaction with surfaces underpins a huge range of processes, from the industrial manufacture of chemicals to developing a hydrogen economy. Understanding collisions of hydrogen with surfaces at a fundamental, molecular level therefore has great value. One property of ground-state H2 that it was particularly difficult to control was its rotational orientation with respect to the surface, which classically corresponds to whether it is rotating like a helicopter (rotational plane parallel to the surface) of like a cartwheel (rotational plane perpendicular to the surface).Using a unique magnetic molecular interferometry technique [1], which combines homogeneous and inhomogeneous magnetic fields, we can control and manipulate the rotational orientation of the H2 molecule before it collides with a surface, and explore what effect it has on the outcome of the molecule-surface collision. In this presentation I will introduce the MMI technique and present results from recent elastic scattering measurements [2,3], before discussing how the technique can be extended to also study the dissociation of H2 when it collides with a surface.

Figure 1: Photo of the experimental apparatus used to perform magnetic molecular interferometry measurements.

A temperature-programmed X-ray photoelectron spectroscopy (TP-XPS) study of tetraphenyl porphyrin on Cu(111)

Clarke M[1], Frampton E[2], Edmondson M[1], Bradford J[1], Gray A[1], Warwick L[1], Saywell A[1]
[1]University of Nottingham, Physics and Astronomy Department, [2]MAX IV Laboratory

Contributed speaker 3 - Michael Clarke, March 31, 2025, 14:50 - 15:10

Halogenated porphyrins on metallic surfaces undergo a surprising variety of reactions when heated, such as ring-closing, metalorganic coordination, self-metalation, and of particular interest here, Ullmann-type coupling. These reactions are known to be influenced by various factors, including porphyrin and substrate chemistry.[1] Porphyrins are of interest as precursor monomers in on-surface assembly, due to their tuneable optoelectronic and gas absorption properties.[2] Here, we detail the reaction of brominated tetraphenyl porphyrin (BrxTPP, x=0-4) on Cu(111), via near edge X-ray absorption fine structure (NEXAFS), X-ray photoelectron spectroscopy (XPS) and scanning tunnelling microscopy (STM). Building upon our previous work, [3,4] temperature programmed XPS (TP-XPS) provides a detailed characterisation of the molecule, obtained as the reaction progresses. Using Arrhenius analysis, we are able to provide insight into the kinetic properties and two-step nature of the dehalogenation reaction.

[1] L. Grill, S. Hecht, Nat. Chem. 12, 115–130 (2020)
[2] E. Vesselli, J. Phys. Mater. 3, 022002 (2020)
[3] M. Edmondson, E. S. Frampton, C. J. Judd, N. R. Champness, R. G. Jones and A. Saywell, Chem. Commun., 2022, 58, 6247–6250.
[4] E.S. Frampton, M. Edmondson, C. J. Judd, D.A. Duncan, R.G. Jones, A. Saywell, Inorganica Chim. Acta, 558, 121718, (2023)

Mind the Gap: In situ XPS/XAS of Co Fischer-Tropsch synthesis at 4 bar

Cong P[1], Gibson J[1,2], Jones E[1], Perez-Dieste V[3], J. Villar-Garcia I[3], Liu L[1], Weatherup R[1]
[1]Department Of Materials, University Of Oxford, [2]School of Chemistry, University of Edinburgh, [3]ALBA Synchrotron Light Source

Contributed speaker 21 - Peixo Cong, April 2, 2025, 10:00 - 10:20

Fischer−Tropsch synthesis (FTS) is critical as an industrial process for converting synthesis gas into higher hydrocarbons.[1] Commercially, FTS is generally performed over cobalt- and iron-based heterogeneous nanoparticle (NPs) catalysts. Since the initial reports by Fischer and Tropsch over a century ago, the underlying mechanism of FTS has remained a subject of ongoing debate, particularly concerning the nature of the active catalytic phase. A key factor in elucidating the reaction mechanism, as well as understanding catalyst activity and selectivity, is the identification of cobalt phases present under reaction conditions.

In this work, FTS is investigated over cobalt NP catalysts using combined in-situ X-ray photoelectron spectroscopy (XPS) and total electron-yield X-ray absorption spectroscopy (TEY-XAS). These soft X-ray techniques offer valuable insights into changes in the metal oxidation state and the surface intermediate species present. However, their shallow probing depth poses limitations in signal collection at elevated gas pressures. Recently, we have demonstrated, for the first time, the capability to perform combined XPS and soft X-ray TEY-XAS measurements at a gas pressure of 4 bar. This is achieved using a customised flow cell2 equipped with graphene windows that provide X-ray and electron transparency. As shown in Fig 1, this allows us to observe markedly different behaviour of Co NP catalysts when exposed to a high-pressure gas environment, more comparable to industrially relevant conditions.

[1] Price, S. et al. Sci. Adv. 2017, 3, e1602838.
[2] Swallow, J et al. J. Am. Chem. Soc 2023, 145, 6730−6740

Influence of Battery Electrode Chemistry on Electrolyte Decomposition

Dettmann L[1], Colbin L, Naylor A
[1]Uppsala University

Contributed speaker 25 - Lasse Dettmann, April 2, 2025, 12:30 - 12:50

A stable solid-electrolyte-interphase (SEI) is essential for performance and durability in rechargeable batteries.[1] While extensive studies have focused on electrolyte-driven SEI formation, the influence of electrode materials remains underexplored.[2] This study examines SEI formation on carbonaceous (glassy carbon), semiconducting (silicon), and metallic (copper) electrodes in model battery systems. Using electrochemical techniques such as linear sweep voltammetry (LSV) and chronoamperometry (CA), combined with hard X-ray photoelectron spectroscopy (HAXPES), we investigate the nucleation of SEI components as a function of surface material and potential. Additionally, we assess the impact of alkali metal cations (lithium vs. sodium) on SEI composition. Our results demonstrate that SEI formation is highly dependent on electrode material, reduction potential, and alkali cation, reinforcing its non-universal nature. These insights underscore the necessity of understanding SEI formation mechanisms when developing advanced electrode materials for next-generation batteries.

[1] S. K. Heiskanen, J. Kim, B. L. Lucht, Joule 2019, 3, 2322–2333.
[2] M. Gauthier, T. J. Carney, A. Grimaud, L. Giordano, N. Pour, H.-H. Chang, D. P. Fenning, S. F. Lux, O. Paschos, C. Bauer, F. Maglia, S. Lupart, P. Lamp, Y. Shao-Horn, J. Phys. Chem. Lett 2015, 6, 5.

Characterisation of topological defects in graphene grown by bottom up synthesis

Klein B[1,2], Stoodley M[1,2], Deyerling J[3], Rochford L[1,4], Morgan D[2], Hopkinson D[1], Sullivan-Allsop S[5], Eratam F[1], Sattler L[6], Weber S[6], Hilt G[6], Generalov A[7], Preobrajenski A[7], Liddy T[1,8], Williams L[1,9], Lee T[1], Saywell A[8], Gorbachev R[5], Haigh S[5], Allen C[1,10], Auwärter W[3], Maurer R[1], Duncan D[1]
[1]Diamond Light Source, [2]University of Warwick, [3]Technical University of Munich, [4]University of Cambridge, [5]University of Manchester, [6]Carl von Ossietzky University Oldenburg, [7]MAX IV Laboratory, [8]University of Nottingham, [9]University of Glasgow, [10]University of Oxford

Contributed speaker 12 - David Duncan, April 1, 2025, 10:40 - 11:00

Introducing defects into graphene often requires post-processing, e.g. by ion sputtering or plasma etching. We present a bottom-up synthesis method yielding graphene with incorporated topological defects on a copper substrate. In the chemical vapour deposition process we use an aromatic precursor that contains the same structural elements as the desired defect. During the growth of the graphene lattice, the topology of the precursor is partly retained and topological defects are formed in the carbonaceous network. In addition to presenting the atomistically resolved non-contact atomic force microscopy (nc-AFM) and aberration correction scanning tunnelling electron microscopy (AC-STEM) that demonstrates this retention of topology, we also present spectroscopic studies into the defective graphene using the techniques of normal incidence X-ray standing waves (NIXSW), near edge X-ray absorption fine structure (NEXAFS) and X-ray photoelectron spectroscopy (XPS) with supporting density functional theory calculations, to elucidate the structural and chemical changes induced by varying defect concentration.

Multi-technique characterization of rhodium single atoms as dicarbonyls on TiO2(110)

Eder M[1], Lewis F[1], Sombut P[1], Hütner J[1], Hao M[1], Rath D[1], Balajka J[1], Pavelec J[1], Libisch F[1], Parkinson G[1]
[1]TU Wien

Contributed speaker 9 - Moritz Eder, March 31, 2025, 17:40 - 18:00

Single-atom catalysts (SACs) have garnered significant attention in recent years due to their potential to minimize noble metal usage by isolating active atoms on metal (oxide) surfaces. However, stabilizing these single atoms remains a major challenge. Ligands, such as carbon monoxide, can stabilize single atoms by transforming them into surface-bound metal complexes, closely resembling the well-defined species in homogeneous catalysis.

In this contribution, we present a comprehensive characterization of a ligand-stabilized single atom: a rhodium gem-dicarbonyl ($Rh(CO)_2$) bound to rutile $TiO_2(110)$. Using XPS, TPD, scanning probe, and a newly developed IRRAS apparatus, we provide a detailed analysis of these sites. Our findings are contextualized through comparisons with theoretical models, containing both established DFT as well as newly developed embedding methods, and insights from powder catalyst studies in the literature. This work demonstrates that multi-technique approaches are essential for the accurate characterization of single-atom catalysts, offering a deeper understanding of their structure and stability.

ME acknowledges funding from the EU Marie Skłodowska-Curie Actions of Horizon-MSCA-2022-PF-01 (Project 101103731 - SCI-PHI).

N-Graphene Defects on Cu(111) by Chemical Vapour Deposition

Eratam F[1], Stoodley M[1,2], Klein B[1,2], Rochford L[1], Clarke M[3], Straw J[3], Warwick L[3], Goto F[4], Williams L[5], Grinter D[1], Lee T[1], Preobrajenski A[6], Vinogradov N[6], Appelfeller S[6], Saywell A[3], Maurer R[2], Duncan D[1,3]
[1]Diamond Light Source, [2]University of Warwick, [3]University of Nottingham, [4]Polytechnic University of Milan, [5]University of Glasgow, [6]Max IV

Contributed speaker 11 - Fulden Eratam, April 1, 2025, 10:20 - 10:40

Nitrogen doping of graphene is a popular approach to tailor the electronic and catalytic properties of graphene, paving the way for various potential applications such as in opto-electronics [a], gas sensing [b] and single atom catalysis [c]. We have fabricated N-doped graphene from the bottom-up using chemical vapour deposition of polyaromatic N-containing precursors, onto a hot Cu(111) surface under UHV conditions. Namely, we have used metallophthalocyanines (MPc: FePc and TiOPc), free-base phthalocyanine (2H-Pc), free-base tetraphenyl porphyrin (2H-TPP) and azabenzopyrene (ABP) [d,e]. By a combination of X-ray photoelectron spectroscopy, density functional theory and normal incidence X-ray standing waves, we have characterised these films with the aim of identifying the presence of graphitic, pyrrolic and pyridinic N defects. Herein, the talk will focus on how we have identified these N defects, as well as the continued challenges in spectroscopically discriminating between the pyridinic and pyrrolic defects.

a) Academic Press, 2018. 103-155.
b) Sci Rep 11, 20719 (2021).
c) Carbon 174 (2021): 772-788.
d) Inorganica Chimica Acta 557 (2023): 121679.
e) Chem. Commun., 2020,56, 3681-3684.

Multimodal Microscopy of Metal Halide Perovskite Thin Films and Devices

Frohna K

Invited speaker 8 - Kyle Frohna, April 1, 2025, 15:50 - 16:20

Metal-halide perovskites are an ever-growing class of materials that have shown remarkable success in optoelectronic applications such as solar cells, light emitting diodes and photodetectors. Contrary to established solar cell technologies such as silicon, perovskite devices are typically thin film and polycrystalline. Perovskite thin films, and devices comprised thereof, exhibit remarkable levels of microscopic disorder in their structure, chemistry and morphology1. This disorder has profound impacts on the properties2, performance and long term stability of these materials. Understanding the disorder of perovskite thin-films and their interfaces with contact layers is critical to the rational improvement of these devices.

In this talk, I will discuss the development and application of a multimodal microscopy toolkit designed to probe the interplay between structural, chemical and optoelectronic properties3,4. We utilise wide-field, hyperspectral, optical microscopy to probe voltage and reflection losses within perovskite films. Spatially correlating these optoelectronic observations with nanoprobe hard X-ray diffraction and fluorescence, we relate nanoscale variations in chemistry and structure to changes in optoelectronic performance. In perovskite films, we find that stochastic, nanoscale chemical variation in composition, baked in upon film formation, creates energetic gradients that charge carriers move upon3. Charge carriers funnel onto high quality, low bandgap regions away from trap states that would otherwise cause power losses. These results help explain how these materials can tolerate such high levels of disorder.

We extend this toolkit to full devices by employing voltage dependent luminescence imaging – a technique that allows us to recreate full current-voltage curves at each spatial point –giving us access to both voltage and current losses at the interfaces with the contacts5. We find that full devices can tolerate large chemical disorder, but variations in current extraction efficiency are much more harmful. Minimising current extraction disorder at the interfaces is shown to be a strong predictor of both higher performance and more stable devices.

1. Tennyson, E. M., Doherty, T. A. S. & Stranks, S. D. Nat. Rev. Mater. 4, 573–587 (2019).

2. Doherty, T. A. S. et al. Nature 580, 360–366 (2020).

3. Frohna, K. et al. Nat. Nanotechnol. 17, 190–196 (2022).

4. Tennyson, E. M. et al. ACS Energy Lett. 6, 2293–2304 (2021).

5. Frohna, K. et al. Nat. Energy (2024) doi:10.1038/s41560-024-01660-1.

Electronic Structure and Surface Dynamics of Fluorine-Induced Defects on Silicon

Ginzburg S[1], Jenkins S[1]
[1]University Of Cambridge

Contributed speaker 16 - Samuel Ginzburg, April 1, 2025, 12:50 - 13:10

Recent first-principles molecular dynamics investigations into radical-mediated oxygen difluoride adsorption on the monohydrogenated Si{001} (2x1) surface [1] revealed the formation of a cationic Si-H-Si bridge motif, consistent with three-centre two-electron bonding. A complementary anionic Si-Si-F motif was also identified, consistent with three-centre four-electron bonding. Building on this work, we have performed first-principles electronic structure calculations and additional molecular dynamics simulations to explore in detail these and other fluorine-induced surface defects on the same surface.

Our results reveal distinct localised defects within the band gap and metastable states that arise upon charge variation. We characterise these defects via computed band structures and vibrational densities of states, and discuss their implications for the possible surface transfer doping of silicon thin-films.

[1] Thake, H., & Jenkins, S.J. Role of Radicals in the Reaction of Oxygen Difluoride with Monohydrogenated Silicon. Phys. Chem. Chem. Phys. 27, 660-671 (2025).

Operando study of salt-assisted WS2 growth

Guan S[1], Yang J, Hofmann S, Rimmer M, Haigh S
[1]University Of Cambridge

Contributed speaker 10 - Shaolian Guan, April 1, 2025, 10:00 - 10:20

Salt enhanced chemical vapor deposition of WS2 and related 2D materials is widespread, and while many mechanisms including vapor–liquid–solid (VLS) mediated growth have been suggested, gaining a more detailed understanding remains challenging. We employ operando scanning electron microscopy to resolve the entire process of salt-assisted CVD of WS2, focusing on a model system of individual, small (<100 µm), sapphire supported sodium tungstate (Na2WO4) salt particles. We reveal support interactions that lead a salt particle to develop a lateral halo interface, driven by surface eutectic melting above 630 °C. This halo dictates the salt wetting as well as Na and W transport, and thus upon gaseous sulfur precursor exposure dominates the spatiotemporal WS2 nucleation and mono- and multilayer domain expansion kinetics. Unlike for a conventional VLS mechanism, large (>20 µm) monolayer WS2 formation does not involve the salt droplet directly attached to the growth facets, rather the salt droplet drives WS2 layer growth in the contiguous halo interface region with a continuous supply of W. We compare this to SiO2 and NaOH treated sapphire where corrosive surface roughening dictates the salt wetting, and critically discuss our findings in the context of the connected wider literature.

Spot Profile Atom-Surface Scattering

Jardine A[1], Radić A, von Jeinsen N, Zhao C, Wang K, Liu B, Lambrick S, Ward D
[1]Cavendish Laboratory, University Of Cambridge

Contributed speaker 15 - Andrew Jardin, April 1, 2025, 12:30 - 12:50

The development of scanning helium microscopy (SHeM) over the last decade has established a consistent capability for high resolution neutral atom imaging of surfaces with resolution down to 100s of nm. The key benefits of the method are exclusive surface sensitivity, a complete elimination of any possibility of beam-induced damage, and new contrast mechanisms.

The emergence of SHeM has also realised the possibility of performing more established helium atom scattering (HAS) type experiments with micron and sub-micron level spatial resolution. Rather than being limited to large area characterization, with results typically averaged over at least a few mm^2, such capability opens up a wide range of new applications. These vary from studying small-grained samples to understanding local variations in surface structure and dynamics.

Here we will review recent experimental results where the microscopic spatial resolution available with new SHeM instruments [1] has been used for spot profile analysis. These include diffraction measurements [2] used to examine the structure of LiF surfaces and 2d materials such as MoS_2, thermal programmed desorption measurements using the helium beam, on 2D materials and other semiconductor surfaces, and measurements of contamination and damage that are indistinguishable with other techniques.

Finally, we will describe how the community can access these techniques, through the new CORDE facility at the University of Cambridge [3].

[1] Chenyang Zhao et al., Vacuum 234, 114006 (2025).
[2] Nick A. von Jeinsen et al., Physical Review Letters 131, 236202 (2023).
[3] CORDE (Collaborative R&D Environment), https://corde.phy.cam.ac.uk

Adsorption Dynamics of Strong Oxidants at a Monohydrogenated Silicon Surface

Thake H, Jenkins S[1]
[1]University Of Cambridge

Contributed speaker 8 - Stephen Jenkins, March 31, 2025, 17:20 - 17:40

We report on first-principles molecular dynamic simulations of the adsorption mechanism for various strong oxidants at the monohydrogenated Si{001} surface. After briefly reviewing earlier work involving ozone (O_3) [1] and molecular fluorine (F_2) [2] we focus mainly upon the adsorption of oxygen difluoride (OF_2) [3] and chlorine trifluoride (ClF_3). We find that OF_2 adsorption is mediated by a transient oxygen monofluoride (OF) radical and results in the formation of characteristic surface defects of Si-H-Si, Si-Si-F, and Si-O-Si type. Adsorption of ClF_3 is much more varied in its outcomes, but typically results in desorption of chlorine monofluoride (ClF) and induces surface defects of Si-H-Si, Si-Si-F, and Si-F-Si type. Implications for semiconductor surface cleaning, etching, and doping will also be discussed.

[1] Fink, C. K. and Jenkins, S. J. Radical-Mediated Adsorption: Ozone Oxidation of Passivated Silicon, Surf. Sci. 602, L100-L103 (2008).
[2] Wu, I. Y. H. and Jenkins, S. J. First-Principles Dynamics of Fluorine Adsorption on Clean and Monohydrogenated Si{001}, Langmuir 38, 7256-7271 (2022).
[3] Thake, H. and Jenkins, S. J. Role of Radicals in the Reaction of Oxygen Difluoride with Monohydrogenated Silicon, Phys. Chem. Chem. Phys. 27, 660-671 (2025).

Low temperature oxidation of carbon monoxide on a reconstructed oxide surface

Karagoz B[1], Hu T[2,6], Stenlid J[3,5], Marks K[4], Hu X[5], Stacchiola D[6], Weissenreider J[5], Head A[6]
[1]Diamond Light Source, [2]Stony Brook University, [3]Stanford University, [4]Stockholm University, [5]KTH Royal Institute of Technology, [6]Brookhaven National Lab

Contributed speaker 6 - Burcu Karagoz, March 31, 2025, 16:40 - 17:00

The search for sustainable catalytic processes has spurred interest in earth-abundant metals like copper as alternatives to precious metal catalysts [1]. This work presents combined experimental and computational results of CO reacting with highly active O atoms on the reconstructed $Cu_2O(111)$ surface at cryogenic temperatures. We observe spectroscopically the formation of carbon dioxide when the (111) facet of a cuprous oxide single crystal is exposed to CO at cryogenic temperatures. Infrared reflection absorption spectroscopy (IRRAS) reveals that CO adsorbs on Cu^{1+} sites and reacts with surface oxygen to form CO_2 without the need for metallic sites, an observation corroborated by isotopic labeling experiments. IRRAS also shows that CO bonds to the surface perpendicularly while CO_2 is tilted approaching a parallel orientation on $Cu_2O(111)$. Sum-frequency generation (SFG) spectroscopy confirms CO adsorption and reveals its thermal desorption between 150 K and 230 K on $Cu_2O(111)$. High-resolution X-ray photoelectron spectroscopy (XPS) provides quantitative insights into surface coverages and oxidation states, showing CO and CO_2 desorption below room temperature. Comparative studies show that the $Cu_2O(100)$ surface does not facilitate CO oxidation under similar conditions, highlighting the structure-sensitive nature of the reaction. Density functional theory (DFT) calculations provide mechanistic insights, indicating that oxygen atoms at the Cu_4O clusters of the nanopyramidal surface reconstruction serve as reactive sites and form CO_2 with minimal energy barriers. This study demonstrates that an oxide, in this case of an earth-abundant metal, can provide highly reactive multifunctional sites, enabling both adsorption and reaction fundamental steps towards the efficient conversion of chemicals. With an understanding that some surface atoms are significantly more reactive than others, design strategies to optimize the number and regenerate these atoms should follow.

References

1. R. M. Bullock, J. G. Chen, L. Gagliardi, P. J. Chirik, O. K. Farha, C. H. Hendon, C. W. Jones, J. A. Keith, J. Klosin, S. D. Minteer, R. H. Morris, A. T. Radosevich, T. B. Rauchfuss, N. A. Strotman, A. Vojvodic, T. R. Ward, J. Y. Yang, Y. Surendranath, Using nature’s blueprint to expand catalysis with Earth-abundant metals. Science 369, eabc3183 (2020).

Research Highlights from the Cambridge Atom Scattering Facility

Kelsall J[1], Radić A[1], Liu B[1], von Jeinsen N[1], Ward D[1]
[1]University Of Cambridge

Contributed speaker 13 - Jack Kelsall, April 1, 2025, 11:50 - 12:10

I will discuss recent research highlights from the Cambridge Atom Scattering Facility, part of CORDE at the University of Cambridge.

One of three instruments that the facility houses, the 3He spin-echo spectrometer (3HeSE) enables measurements of surface dynamics from picoseconds to several nanoseconds thanks to its ultrahigh, sub-μeV energy resolution. I will highlight recent work regarding the diffusion of S/Ni(111) at near-ambient temperatures, in which there is significant islanding around surface defects. The results aid the understanding of how sulphur impurities cause embrittlement in nickel and similar metals. 3HeSE also enables measurements of low-energy phonons, while the high energy resolution makes it possible to determine phonon linewidths and lifetimes, an understanding of which is vital for improving thermal transport. I will touch upon recent studies that have categorised phonon interactions with electrons, other phonons and defects, including work demonstrating that electron-phonon interactions dominate unexpectedly in Ru(0001) [1]. I will also describe recent studies into non-metallic samples such as MoS2, single-crystal perovskites and bulk hBN.

The facility houses two helium atom microscopes, which offer non-damaging imaging with sub-micron resolution and unique contrast mechanisms. The capability of the instruments has been expanded to include 'microdiffraction', in which diffraction scans are obtained from micron-sized spots on the surface. The examples of LiF and MoS2 will be discussed [2]. The methodology has broad relevance for studying technological and polycrystalline samples. Otherwise, the high surface sensitivity of SHeM enables the imaging of biofilms, which are challenging to visualize with optical methods, broadening the range of delicate biological samples that can be studied using the technique.

[1]: B. Liu et al., Phys. Rev. Lett., 2024 [2]: N. A. von Jeinsen et al., Phys. Rev. Lett., 2023

4He and 3He – 4He mixture films studied by neutron reflectometry

Kirichek O[1]
[1]Isis Facility, Stfc, Ukri

Contributed speaker 19 - Oleg Kirichek, April 1, 2025, 15:10 - 15:30

In the quantum world superfluid helium 4He can defy gravity and is able to climb out of any container in a thin film that moves with such a pace that the container is drained in minutes. However, of the many quantum fluid systems superfluid helium films remain one of the most elusive for experimental investigation.

Here we present a study of pure 4He and 3He/4He mixture films using specular neutron reflection, in the temperature range of 150 mK to 1.5 K [1]. Thanks to the exceptional sensitivity and precision of this technique, we have observed a phase-separated 3He/4He mixture film at 170 mK. Then we have been able to watch the gradual dissolution of its 3He top layer into 4He with increasing temperature, in agreement with current theories. Furthermore, the surprising behaviour of the helium mixture at 300 mK hints at the possibility of an as-yet unstudied geometrically restricted phase transition. The subsequent restoration of the layered structure at 1.5 K was equally unexpected.

We also developed a sample environment application based on the surprising behaviour of the helium mixture at 300 mK. In neutron scattering powder diffraction experiments the helium exchange gas is often loaded into the experimental cell to thermalize the sample. We have used destruction of 3He/4He mixture film at 300 mK to reduce the heat flow through the filling capillary.

[1] O. Kirichek, et al. Commun. Phys. 7, 181 (2024).

Indium-silver surface alloy explored using photoelectron microscopy and spectroscopy

Laverock J[1], Mason T[1], Dugdale S[1]
[1]University Of Bristol

Contributed speaker 4 - Jude Laverock, March 31, 2025, 15:10 - 15:30

Indium-silver alloys have recently attracted attention as high performance thermal interface materials in high power semiconducting devices, which are rapidly becoming crucial in the thermal management of modern artificial intelligence computing architectures, and as bimetallic nanoparticles for sensor applications.

Here, indium deposited on Ag(111) is investigated via photoelectron microscopy and spectroscopy to reveal its surface structure and electronic behaviour at the Bristol Ultraquiet NanoESCA Laboratory (BrUNEL). Careful X-ray photoelectron spectroscopy (XPS) measurements of the scattered electron spectrum are used to accurately extract both the alloy composition and thickness as a function of the nominal indium flux (deposition time). The indium layer is found to spontaneously form a self-limiting alloy with silver up to a few nanometres thick at room temperature.

Subsequent spatially-resolved micro angle resolved photoemission spectroscopy (µARPES) and low-energy electron diffraction (µLEED) experiments, performed at BrUNEL and Diamond Light Source, demonstrate the In-Ag alloy is coherent with the Ag substrate, and that the In atoms are substitutionally disordered within the Ag FCC lattice. µARPES was recorded using both monochromatic He I (21.2 eV) and monochromatic Ar I (11.6 eV) light sources, yielding different information depths. The experimental results are discussed through comparison with density functional theory (DFT) calculations within the coherent potential approximation (CPA) to model the disorder.

Accurate core electron binding energies from ab initio calculations

Lischner J

Invited speaker 10 - Johannes Lischner, April 2, 2025, 09:30 - 10:00

Abstract: X-ray photoemission spectroscopy (XPS) measures the binding energies of core levels. As these binding energies are highly sensitive to the local chemical environment, XPS is a powerful technique for gaining insights into the structure of complex materials. However, the analysis of measured XPS spectra can be challenging as it is often difficult to infer the chemical environments from the measured binding energies. To address this problem, my research group has developed accurate parameter-free modelling approaches which can predict absolute core electron binding energies of molecules, solids (both metallic and insulating) and surfaces. These approaches are based on density-functional theory and the Delta-SCF technique and often produce absolute binding energies with errors of less than 0.2 eV.

Characterization of defect-induced acoustic surface phonon linewidth broadening using helium spin echo

Liu B[1]
[1]Cavendish Laboratory, University of Cambridge

Contributed speaker 14 - Boyao Liu, April 1, 2025, 12:10 - 12:30

In metals, thermal conductivity is influenced by phonon lifetimes; in semiconductors and insulators, thermal conductivity is almost exclusively determined by phonon lifetimes. Hence the interaction between defects and phonons is crucial for thermal management in all materials, which is a pressing issue in many fields of science and technology. For example, in the fast moving microelectronics industry, the development of high density electronic devices has brought huge advances in computational capability, in turn enabling huge societal benefits. Nevertheless, the intense levels of heat dissipation in such devices bring major challenges and ultimately limit performance. New device architectures, e.g. based on 2D materials, are currently of great interest as they have the prospect to address these demands, as well as to lower overall power consumption [1]. Typically, phonons are the major heat carriers in all these devices, so defects are a main factor that affects their thermal performance [2].

There have been great efforts to investigate defect-phonons interactions [3]. Most important in the present context is the influence of defects on acoustic phonon lifetimes (inversely proportional to linewidth), which determines the thermal conductivity. However, acoustic phonon lifetime shortening induced by defects is extremely challenging to measure; direct experimental observation is still lacking, especially in 2D systems, and so far the issue has mainly been explored through theoretical calculations and computer simulations [4].

In the present work, the first direct measurement of the influence of crystal defects on the acoustic phonon lifetime on a Ni(111) surface is presented [5]. The changes in the RW mode phonon linewidth was measured using the helium spin echo (HeSE) technique. HeSE harnesses the nuclear spin of helium-3 atoms to probe energy transfer during scattering from surfaces. With precise control of the nuclear spin, the energy resolution of HeSE can reach unprecedented μeV levels [6]. With the HeSE technique, the energy linewidth of phonons can be resolved, allowing us to access information on defect-phonon interactions.

In this work, the changes in the RW mode phonon linewidth were measured using HeSE, while the surface defect density was tuned using argon ion sputtering and annealing. This work will show that the phonon lifetimes vary with momentum and decrease with surface defect density due to defect-phonon scattering, which enables a quantitative estimate of coupling between the RW mode and surface defects [5].

[1] M. Chhowalla, D. Jena, H. Zhang, Two-dimensional semiconductors for transistors, Nature Reviews Materials, 1 (2016) 16052.
[2] X. Qian, J. Zhou, G. Chen, Phonon-engineered extreme thermal conductivity materials, Nature Materials, 20 (2021) 1188-1202.
[3] X. Yan, C. Liu, C.A. Gadre, L. Gu, T. Aoki, T.C. Lovejoy, N. Dellby, O.L. Krivanek, D.G. Schlom, R. Wu, X. Pan, Single-defect phonons imaged by electron microscopy, Nature, 589 (2021) 65-69.
[4] B. Mortazavi, S. Ahzi, Thermal conductivity and tensile response of defective graphene: A molecular dynamics study, Carbon, 63 (2013) 460-470.
[5] B. Liu, J. Kelsall, D.J. Ward, A.P. Jardine, Experimental Characterization of Defect-Induced Phonon Lifetime Shortening, Physical Review Letters, 132 (2024) 056202.
[6] A.P. Jardine, H. Hedgeland, G. Alexandrowicz, W. Allison, J. Ellis, Helium-3 spin-echo: Principles and application to dynamics at surfaces, Progress in Surface Science, 84 (2009) 323-379.

Surface Study of Structure Evolution and Deactivation of Gauze Catalysts for Nitric Acid Production

Ma Y[1], Wang R[1], Wilson M[2]
[1]University College London, [2]Johnson Matthey

Contributed speaker 22 - Yining Ma, April 2, 2025, 10:20 - 10:40

Nitric acid (HNO_3) ranks 10th in global chemical production and is synthesized by oxidizing ammonia (NH_3) to nitric oxide (NO) and then to nitric acid, with NO selectivity being key for efficient nitrogen utilization. However, surface oxidation and dendrite formation on commercial PtRh and PtRhPd alloy gauzes create complex morphological and compositional changes, impacting NO yield.[1]

To explore the reconstructing mechanism, we have conducted SEM (Scanning Electron Microscope), XANES (X-ray Absorption Near Edge Structure), XRF (X-ray Fluorescence) analysis on PtRh and PtRhPd gauzes with different compositions and aging times. The gauze wire was fixed in resin and cut into thin slices to obtain the cross-sectional area.

In SEM analysis dendrite formation was observed on the aged sample compared to a fresh, smooth gauze, Fig 1.a and b. A preliminary X-ray transmission map was taken at 11521 eV (Fig. 1c), which showed low X-ray transmission over the bulk of the sample due to the thickness of the gauze wire (blue colour). Comparatively, red colour shows the voids, with yellow and green colours showing dendrites formed on the surface. For XRF cross section mapping in Fig.1 d and e low levels of rhodium aggregation was observed, with more rhodium oxidation at the surface/dendrite part on the cross-section than the bulk. Meanwhile, average Rh L3 XANES spectra for bulk and dendrite parts of the cross section showed a similar change in oxidation state between the two regions.

[1] Liu, X.; Han, Y.; Jia, H. Rare Metal Materials and Engineering 2017, 46, 339-343.

Forces Driving Chirality Transfer on a Metal Surface

McBreen P[1], Zahidi E[1], Dong Y[1], Hammer B[2]
[1]Laval University, [2]Aarhus University

Contributed speaker 2- Peter McBreen, March 31, 2025, 14:30 - 14:50

Control of enantioselection is an especially demanding challenge in heterogeneous catalysis and its study explores phenomena ranging from ligand-induced rate-enhancement to the interplay between chemisorption and intermolecular forces in determining the structure and dynamics of chirality-transfer complexes. In this study, a combination of STM, DFT and reflectance-IR data is used to define the structure of individual complexes, the intermolecular interactions involved, the activation of prochiral functional groups, and complexation state changes within isolated complexes. Although the studies are carried out on model systems under vacuum conditions, the observed phenomena are largely consistent with the operando heterogeneous asymmetric catalysis literature. Emphasis will be placed on the three most important insights gained from studies of single complexes formed by chiral modifiers and prochiral reactants on Pt(111): (i) complexation is driven by multiple attractive non-covalent interactions; (ii) weak non-covalent interactions play a determining role in stereodirection; (iii) precursor state dynamics are key to forming privileged complexation structures. The studies also show that DFT calculations perform well in predicting the structure and dynamics of individual chemisorbed chirality-transfer complexes.

Hybrid plasmons at Nano-carbon/Topological-Insulator interfaces characterised with STEM-EELS

Moorsom T[1], McCaley M[2], MacLaren D[2], Nizamuddin Bin Muhammad Mustafa A[3], Ramadan S[3], Petrov P[3], Burton J[1], Sasaki S[1], Knox C[1], Rogers M[1], Ramasse Q[4], Ansari L[5], Gity F[5], Hurley P[5]
[1]University Of Leeds, [2]University of Glasgow, [3]Imperial College London, [4]SuperSTEM, [5]Tyndall National Institute

Contributed speaker 17 - Timothy Moorsom, April 1, 2025, 14:30 - 14:50

A major barrier to the development of practical plasmonic devices is electronic scattering. [1] However, low dimensional systems including graphene offer high mobility and low scattering rates, making them attractive for the development of plasmonic devices. [2] Topological insulators are especially interesting for operation at both THz and optical frequencies [3] because of their topologically protected surface states (TSS). Practical TI-based plasmonic devices will require a means of tunable control of 2D plasmons. One approach is to dope the surface with impurities to create a 2D electron gas (2DEG). [4] However, these dopants are extremely reactive, so the effect is unstable outside ultra high vacuum. A more robust alternative is the use of thin films of organic molecules and dyes. [5] The ultimate goal is to find a stable molecular thin film that supports reversible charge transfer to an underlying TI. [6] Electron Energy Loss Spectroscopy (EELS) provides a useful probe of localised surface effects where interfacial electronic structure can be mapped with sub-nm resolution. In particular, the 2D π plasmon mode observed in both topological interfaces and 2D materials such as graphene provides a sensitive probe of 2D confined surface states. [7] We have found that C60 forms highly ordered crystals on TI surfaces at very low deposition energy, producing atomically sharp interfaces that are free from structural defects and stable to degradation. C60 was chosen for its high electron affinity, resulting in significant charge transfer from the TI interface. Using STEM-EELS and momentum resolved EELS (QEELS) we have performed a high resolution study of the plasmonic excitations in Bi2Se3/C60 heterostructures with sub-atomic resolution in the opitcal and UV regime. We have demonstrated that there are fundamental differences in the pi states at the interface between a TI and trivial insulator, and an interface between a TI and a molecular film. These manifest as differences in band bending and 2D confinement of the surface states, as well as changes in the dispersion relation of the pi plasmon. This shows that molecular layers profoundly change the surface behaviour of TIs. [8]

Figure 1 - a. STEM-BF image of Bi2Se3/C60 interface. b. DFT model of interfacial charge transfer. c. Low-loss EELS spectra recorded at various positions across the interface. d. STEM-EELS maps across different energy windows, capturing different surface and bulk excitations in the heterostructure.

[1] - J B Khurgin and G Sun, andau Damping—The Ultimate Limit of Field Confinement and Enhancement in Plasmonic Structures, pp. 303–322. Springer, Cham (2017).
[2] - D A Iranzo et al, Science, 360, 6386, 2018.
[3] - Y P Lai et al, Nanomaterials and Nanotechnology, 4, 13, 2014.
[4] - M Bianchi et al, ACS Nano, 6, 8, 2012.
[5] - S Jakobs et al, Nano Letters, 15, 9, 2015.
[6] - T Wei et al, Phys Rev B, 105, 205408, 2022.
[7] - S C Liou et al, Phys Rev B, 87, 085126, 2013.
[8] - M McCauley, et al. arXiv preprint arXiv:2410.23983 (2024).

Timing the Escape of a Caged Electron

Fields C[1], Foerster A[2,6], Ghaderzadeh S[2], Popov I[2], Huynh B[2,5], Junqueira F[1], James T[1], Alonso Perez S[1], Duncan D[2,3], Lee T[3], Wang Y[1], Bloodworth S[4], Hoffman G[4], Walkey M[4], Whitby R[4], Levitt M[4], Kiraly B[1], O'Shea J[1], Besley E[2], Moriarty P[1]

[1]School of Physics and Astronomy, University Of Nottingham, [2]School of Chemistry, University of Nottingham, [3]Diamond Light Source, [4]School of Chemistry, University of Southampton, [5]Dept of Chemistry, University of Oxford, [6]National Institutes of Health

Contributed speaker 18 - Connor Fields, April 1, 2025, 14:50 - 15:10

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. We have applied the core hole clock technique -- an energy-domain variant of ultrafast spectroscopy -- to probe the delocalization of a photoexcited electron inside a closed molecular cage, namely the Ar $2p^5$ $4s^1$ state of Ar@C_{60}. Despite the lack of frontier orbital mixing in the ground configuration, almost 80% of the excited state density is found outside the buckyball due to the formation of a markedly diffuse hybrid orbital. Far from isolating the intracage excitation, the surrounding fullerene is instead a remarkably efficient conduit for electron transfer: we measure characteristic delocalization times of 6.5 ± 0.1 fs and < 0.6 fs, respectively, for a 3D Ar@C_{60} film and a 2D monolayer on Ag(111).

For the endofullerene monolayer, we have combined core hole clock (CHC) spectroscopy with the normal incidence X-ray standing wave (NIXSW) technique to measure the position of the encapsulated Ar atom above the Ag(111) surface. Despite the large value of the Ar-Ag(111) adsorption height (5.55 ± 0.04 Å), Ar 2p photoemission spectra are highly asymmetric and are best fit using a Doniach-Sunjic lineshape consistent with metallic screening -- further strong evidence of "through cage" coupling of the encapsulated argon with the Ag(111) substrate,

Molecular diffusion mimics ``universality classes'' of bursty human dynamics

Moller M[1], Rahe P[2], Moriarty P[1]
[1]University Of Nottingham, [2]Institut für Physik, Universität Osnabrück

Contributed speaker 5 - Philip Moriarty, March 31, 2025, 16:20 - 16:40

Processes involving bursts of activity separated by quiescent periods are so prevalent across spatial and temporal scales in nature that there has been a decades-long search for universal principles that connect these ``bursty'' phenomena. [1] Complex systems and phenomena spanning email traffic to earthquake activity exhibit non-Poissonian, heterogeneous temporal behaviour that has typically, and contentiously [2], been characterised in terms of power-law distributions of inter-event times (with different power law exponents representing distinct "universality classes").

The complexity of social systems makes determining the fundamental origin of their bursty dynamic behaviour exceptionally challenging at best. We have instead selected a highly simplified, and thus rather more tractable, bursty process: molecular diffusion on a surface (namely perylene-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) on Ag(110)), monitored using the tip of a scanning tunnelling microscope (STM). Sporadic pulses in the tunnel current signal result when a PTCDA molecule diffuses underneath the STM tip [3].

Inter-arrival time distributions for molecular diffusion monitored in this way show intriguing parallels with those previously observed for a variety of social processes (including email communication, web browsing, library loans [1]). We shall discuss the origin of these parallels and explore whether molecular transit times can indeed be described within the same "universality class" as other bursty processes such as email correspondence.

[1] EG Altmann, arxiv.org/abs/2407.19874; A-L Barabasi, Nature 435 207 (2005)
[2] R Dean Malmgren, et al., Science 325 1696 (2009); E Keller-Fox BioEssays 27:1060 (2005)
[3] S. Hahne, et al., Phys. Rev. B 87, 085409 (2012) and references therein

Ultrafast Optical and Terahertz STM of Light-Induced Processes at Solid Surfaces

Müller M

Invited Speaker 2 - Melanie Mueller, March 31, 2025, 13:40 - 14:10

The integration of broadband optical and terahertz (THz) radiation with low-temperature scanning tunneling microscopy (STM) has opened up new possibilities for probing ultrafast processes and the optical response of surfaces at the atomic scale [1]. I will introduce two modes of ultrafast STM - optical photon-driven STM (ph-STM) and THz-lightwave-driven STM (THz-STM) - which allow for the probing of light-induced and ultrafast processes at surfaces with simultaneous femtosecond temporal and nanometer to angstrom spatial resolution. As a first example, I will discuss the capabilities of ph-STM for the local detection of coherent phonon (CP) dynamics in ultrathin ZnO films on Ag(111) [2]. Here, the optical resonance of the ZnO/Ag(111) interface plays a crucial role in the efficient detection of CPs via the photoinduced tunneling current, which we further explore using the recently developed two-color pump-probe ph-STM. In another study, we use THz-STM to probe the photoinduced dynamics of the charge density wave (CDW) insulator 1T-TaS2 [3]. Upon photoexcitation, we observe a periodic modulation of the tunneling current at a frequency of 2.4 THz, corresponding to the CDW amplitude mode in 1T-TaS2, which can be locally probed by the THz-lightwave-driven tunneling current. Finally, I will briefly outline the next steps and challenges in this vibrant field of STM towards imaging and spectroscopy of light-induced phenomena in complex quantum materials at the atomic scale.

References:
[1] M. Müller, Prog. Surf. Sci. 99, 1 (2024)
[2] S. Liu et al., Sci. Adv. 8, 42 (2022)
[3] L. Parra Lopéz et al. (in preparation)

Single-Atom Catalysis: An Atomic-Scale View

Parkinson G

Invited speaker 3 - Gareth Parkinson, March 31, 2025, 15:50 - 16:20

Over the past decade, single-atom catalysis (SAC) has become a major focus in catalysis research. It is now well established that the catalytic activity of metal atoms is strongly influenced by their interaction with the support material. The role of the local coordination environment has drawn comparisons to metal–organic complexes, fueling excitement about the possibility of fine-tuning SAC by controlling adsorption geometry.Surface science techniques are particularly effective for studying this aspect of SAC, as they allow us to precisely determine metal atom geometries and correlate them with catalytic behavior. In this talk, I will present our recent work on Rh atoms supported on metal oxides, focusing on their interaction with CO, ethylene, and H_2—key reactants in the hydroformylation reaction (alkene + CO + H_2 → aldehyde). Several powder-based SAC systems have already demonstrated activity for this reaction, but the mechanism is not well understood. Here, I will show how the local environment of Rh atoms influences both the adsorption energy of reactants and their ability to adsorb simultaneously. These insights highlight the critical role of atomic-scale structure in optimizing single-atom catalysts.

Atomic structure of epitaxial 2D materials elucidated by Surface X-ray diffraction

Prévot G

Invited speaker 7 - Geoffroy Prevot, April 1, 2025, 14:00 - 14:30

Since the experimental discovery of graphene, thousands of 2D materials have been identified by numerical simulations. However, only a small part of them has been synthesized, most often by exfoliation of the bulk material. Conversely, the epitaxial growth of 2D materials can lead to the formation of new structures differing from those of their bulk counterparts. This is for example the case of silicene, germanene or stanene, which have an electronic structure similar to the one of graphene, but do not form lamellar materials.

For these novel epitaxial 2D monolayers, the knowledge of their atomic structure is a key point for the understanding of their properties (electronic, optical, mechanical, etc.). For this purpose, surface X-ray diffraction is by far the most quantitative method. Indeed, the diffracted intensities measured in reciprocal space are proportional to the squared modulus of the Fourier transform of the electronic density.

In this talk, I will present the classical methods used to retrieve the atomic positions from the diffraction measurements (such as structure refinement with chi-square minimization or analysis of the Patterson map), the recent developments achieved with phase retrieval algorithms, and some perspectives. Examples will be taken from epitaxial silicene and germanene layers recently synthesized on metal substrates, and measured on the SixS beamline of Soleil synchrotron.1–7

Chemical bonding and electronic structure of metal dihydrides explored by hard X-ray photoelectron spectroscopy (HAXPES)

Regoutz A

Invited speaker 11 - Anna Regoutz, April 2, 2025, 11:20 - 12:10

Metal hydrides hold significant promise in various hydrogen-related technologies, encompassing energy storage, hydrogen compression, and hydrogen sensing. Although metal hydrides appear simple compared to many other energy materials, understanding the electronic structure and chemical environment of hydrogen within them remains a key challenge. This work presents a new analytical pathway to explore these aspects in technologically relevant systems using Hard X-ray Photoelectron Spectroscopy (HAXPES) on thin films of two prototypical metal dihydrides: YH2−δ and TiH2−δ.[1,2] By taking advantage of the tunability of synchrotron radiation, a non-destructive depth profile of the chemical states is obtained using core-level spectra. Combining experimental valence band spectra collected at varying photon energies with theoretical insights from density functional theory (DFT) calculations, a description of the bonding nature and the role of d versus sp contributions to states near the Fermi energy are provided. Moreover, a reliable determination of the enthalpy of formation is proposed by using experimental values of the energy position of metal s band features close to the Fermi energy in the HAXPES valence band spectra.

Selected references
[1] C. Kalha, L. E. Ratcliff, G. Colombi, C. Schlueter, B. Dam, A. Gloskovskii, T.-L. Lee, P. K. Thakur, P. Bhatt, Y. Zhu, J. Osterwalder, F. Offi, G. Panaccione, A. Regoutz, “Revealing the Bonding Nature and Electronic Structure of Early-Transition-Metal Dihydrides”, PRX Energy, 3, 013003, 2024, https://doi.org/10.1103/PRXEnergy.3.013003.
[2] C. Kalha, N. K. Fernando, P. Bhatt, F. O. L. Johansson, A. Lindblad, H. Rensmo, L. Zendejas Medina, R. Lindblad, S. Siol, L. P. H. Jeurgens, C. Cancellieri, K. Rossnagel, K. Medjanik, G. Schönhense, M. Simon, A. X. Gray, S. Nemšák, P. Lömker, C. Schlueter, and A. Regoutz, "Hard X-ray Photoelectron Spectroscopy – A Snapshot of the State-of-the-Art in 2020", J. Phys. Condens. Matter, 33, 233001, 2021, https://doi.org/10.1088/1361-648X/abeacd

Ionic liquid-modified perovskite films for enhanced solar cell stability

Tiwari U[1], Cole J[1], Li Z[3], Walton A[2], Dwyer L[2], Spencer B[2], Zlatogorsky S[1], Syres K[1]
[1]University of Central Lancashire, [2]University of Manchester, [3]University of Aarhus

Contributed speaker 20 - Karen Syres, April 1, 2025, 16:20 - 16:40

Halide perovskites have emerged as promising candidates for photovoltaic applications due to their remarkable device efficiencies. Despite this progress, the commercial viability of perovskite solar cells is hindered by their long-term instability under high temperature and humidity. Several strategies have been explored to overcome this, one of which is additive engineering. The interaction between the additive and perovskite results in defect passivation and ion immobilisation, improving device performance and stability.

In this study, we examine the incorporation of ionic liquids [BMIM][BF4] and [BMIM][Cl] into mixed-halide perovskite films. We use X-ray Photoelectron Spectroscopy (XPS), Near Edge X-ray Absorption Fine Structure (NEXAFS), Hard X-ray Photoelectron Spectroscopy (HAXPES) and Near-Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS) to assess their resistance to heat and moisture. In addition, we investigate the role of a SnO2 electron transport layer (ETL) in improving film stability. Our results indicate that the IL-modified perovskite films on SnO2 demonstrate enhanced thermal stability, withstanding temperatures of at least 300 °C. The ionic liquids show different behaviours, with [BMIM][BF4]-modified films showing greater thermal stability and [BMIM][Cl]-modified films showing greater moisture stability. We infer that the combined use of ionic liquids and SnO2 significantly enhances the thermal and moisture stability of perovskite films, advancing their potential for commercial application.

How Defects Freeze Ripples in 2D Materials

Thiemann F

Invited speaker 4 - Fabian Thiemann, April 1, 2025, 09:00 - 09:30

Two-dimensional (2D) materials exhibit nanoscale ripples that fundamentally influence their mechanical, electronic, and chemical properties. Introducing atomic defects is a common strategy to tailor these materials for specific applications, yet understanding the intricate relationship between ripple dynamics and defect characteristics remains challenging. Experimental techniques often lack the necessary resolution to capture the full temporal evolution of ripples across an entire membrane.

In this talk, I will present how machine-learning-driven simulations of graphene, the prototypical 2D material, allow us to probe the connection between ripples and different types of atomic defects. Specifically, we find that above a critical defect concentration, free-standing graphene sheets undergo a transition from freely propagating ripples to static buckling. Our computational approach resolves these dynamics at atomic resolution, revealing that this transition is governed by elastic interactions between defects. The strength of these interactions varies across defect types, and by quantifying their impact using structural and dynamic metrics, we establish a unifying framework for understanding the dynamic-to-static transition in 2D materials.

Our findings help reconcile puzzling experimental observations and open new avenues for designing 2D devices with precisely controlled rippling behaviour, potentially enabling novel applications in nanotechnology.

Metal-mediated exfoliation of 2D materials (2DMs); probing interactions at the Au-2DM interface.

Wilson N

Invited speaker 5 - Neil Wilson, April 1, 2025, 09:30 - 10:00

Metal-mediated exfoliation can give macroscopic (millimetre or more) monolayers of a wide range of 2D materials (2DMs). This is both a useful tool for fabrication, and an interesting opportunity for studying the intricacies of interactions at the interfaces between three-dimensional metals and 2D materials. Understanding these interactions is essential for the integration of 2DM into (opto)electronic circuits as well as for unravelling the mechanism for metal-mediated exfoliation. Here, I will present some of our recent results using template-stripped gold for metal-mediated exfoliation of 2DMs, concentrating on prototypical examples of a 2D semiconductor (WSe2) and a 2D magnet (CrSBr). The large monolayer / few-layer flakes on ultra-flat gold that result from metal mediated exfoliation are ideally suited to study by surface science techniques. We gain insight into the Au-2DM interface through spatially resolved photoemission spectroscopy, at the I05 beamline of Diamond Light Source, both of core levels and angle-resolved of the valence bands. Contrasting results are observed for the two material systems, but both reveal the importance of charge transfer and hybridisation, consistent with covalent like quasi-bonding at the Au-2DM interface.

ISSC 2025 - Poster Presentations

Poster Board no.	First Name	Last Name	Paper Title
1	Nisrin	Alnaim	A Facil Green Synthesis of Moringa Nanoparticles encapsulated PVA matrix for potential Applications
2	Sevinc Yagmur	Bekler	Extending the Pressure Limits of Operando Soft X-Ray Spectroscopies
3	Francesco	Carla	The I07 surface and interface x-ray diffraction beamline
4	Pilar	Ferrer	Surface and bulk structure of nanoparticle spinel ferrites MFe2O4 (M = Co, Cu, Zn) for photocatalysis
5	Tairu	Ge	STM of ultrathin MnxNbyOz nanophases on Au(111)
6	Rodolfo	Hermans	Liquid Brain, Excitable Liquid Interfaces as Computational Substrates for Molecular Characterization
7	Peter	Lebedev-stepanov	Sliding of a liquid spherical droplet in an external insoluble liquid at low Reynolds numbers
8	Faith	Lewis	O_2 Dissociation on α-$Fe_2O_3(1\bar{1}02)$-(1×1)
9	Matthew	Ord	Squeezing of Adsorbates in the Caldeira Leggett Model
10	Amretashis	Sengupta	A first principles study on 2 dimensional Zinc Carbide
11	Eleanor	Teather	Circular dichroism study of alanine on Cu(110) as a model for enantioselective heterogeneous catalysis
12	Amelia G.	Thompson	The adsorption height of nitrogen doped graphene grown by chemical vapour deposition
13	Sparsh	Tyagi	Synthesis and Characterization of Single-Layer Two-Dimensional M2(HITP)3 {M= Ni, Fe} Metal-Organic Frameworks on Au(111)
14	Haozhe	Zhang	Tuning 2D perovskite for photocatalysis

A Facil Green Synthesis of Moringa Nanoparticles encapsulated PVA matrix for potential Applications

Alnaim N[1]
[1]King Faisal University

Moringa oleifera is a good source of antibacterials and antioxidants that can be applied to the food and pharmaceutical industries [1]. Herein, the moringa nanoparticles (MNPs) are encapsulated into polyvinyl alcohol (PVA) by sol-gel method at 70 °C. The morphology of MNPs/PVA film shows spherical nanoparticles with an average particle diameter of 2.02 nm ±0.7 nm. The EDX mapping reveals the uniform distribution of MNPs species into PVA matrix. Fourier transform infrared spectroscopy (FTIR) exhibited the heterogeneous chemical bonding between metal and functional groups. The prepared MNPs/PVA film has potential uses in food packaging and antibacterial coating.

Extending the Pressure Limits of Operando Soft X-Ray Spectroscopies

Bekler S[1], Cong P[1], Weatherup R[1]
[1]University of Oxford, Department of Materials

Heterogeneous catalysis is crucial for industrial chemical synthesis and for reducing global CO_2 emissions. Optimizing catalytic processes requires an in-depth understanding of their mechanisms, which operando measurements can provide by revealing reaction dynamics and intermediates in real time. While soft X-ray photoelectron and absorption spectroscopy (XPS, XAS) are powerful tools for analyzing chemical and electronic states, operando studies at high pressures are challenging due to the short inelastic mean free path of electrons. Recent advances, including differential pumping and environmental cells, have enabled X-ray spectroscopies at atmospheric pressures. We previously developed an environmental cell with a graphene-sealed perforated Si_3N_4 membrane, enabling XPS and XAS measurements at pressures up to 1.5 bar [1].

Suspended graphene membranes are typically prepared by transferring graphene onto perforated supports, but this method can introduce defects and requires considerable experimental skill to minuses cracks and wrinkles [2]. To address this, we develop an approach to directly grow graphene on Si_3N_4 membranes by Chemical Vapor Deposition (CVD), thus avoiding the transfer step. A suspended nickel catalyst layer is deposited onto perforated Si_3N_4 before introducing acetylene precursors at 600–650°C, minimizing damage to the membrane. The Ni layer is then etched away, leaving graphene sealed over the perforations. We demonstrate the success of this approach via leakage tests, Raman spectroscopy, and electron microscopy, and apply it to study CO_2 hydrogenation to methanol on Cu-based catalysts.

1 – Weatherup, R.S. et al. Phys. Chem. Lett. 2016, 7, 9, 1622 – 1627.
2 – Jones, E.S. et al. ChemCatChem 2024, 16(16).

The I07 surface and interface x-ray diffraction beamline

Carla F[1], Rawle J[1], Shao L, Warne A
[1]Diamond Light Source

The I07 beamline at Diamond Light Source is a facility dedicate to the characterisation of surfaces and buried interfaces using x-ray diffraction and scattering techniques in a variety of different sample environments. Thanks to the high flux and high energy (5-30keV) source provided by its undulator the beamline is particularly suitable for in-situ and operando experiments on surfaces and interfaces, which can be performed in conditions ranging from Ultra High Vacuum (UHV) to liquids and high pressure gases (up to 20 bar). The beamline is also largely used for the characterisation of thin films and buried interfaces.

The beamline is equipped with two experimental hutches, the first hosting a multipurpose instrument consisting of a versatile 2+3 circles diffractometer of operating in horizontal and vertical scattering geometry, capable of carrying payload up to 250kg. Different types of sample environments available at the beamline can be installed on the instrument (electrochemical cells, various environmental chambers, high temperature environment, high pressure catalysis reactor, compact UHV chamber) as well as bespoke setups. The system is also coupled with a double crystal deflector that allows to perform diffraction, scattering and reflectivity experiments on liquid surfaces (different Langmuir trough setups are available for this purpose). The second experimental hutch is instead equipped with a 2+3 diffractometer mounting a UHV chamber, that allows for in-situ sample preparation (sputtering/annealing, PVD) and characterization. The system can operate in a base pressure of 10^-10mbar, it is equipped with a number of spare ports for the integration of additional equipment, includes XPS and LEED systems as auxiliary tools for surface characterisation and is connected with a system of leak valves that permits precise dosage of gases.

A versatile system of detectors permits fast data acquisition and can be used to map the reciprocal space at different length scales. Surface dynamics can be also investigated in time-dependent experiment down to the millisecond regime. A fluorescence detector can be also installed on request to perform XAS experiment in parallel with diffraction and scattering experiments, providing additional chemical information.

Surface and bulk structure of nanoparticle spinel ferrites MFe2O4 (M = Co, Cu, Zn) for photocatalysis

Ferrer P[1], Hall C[1,2], Grinter D[1], Held G[1], Grau-Crespo R[2]
[1]Diamond Light Source, [2]University of Reading

Ferrites are metal oxides with the spinel structure, AB2O4, where A represents divalent metal cation (e.g. Co2+, Cu2+, Zn2+) and B represents the trivalent cation, Fe3+. In a normal spinel the A and B cations occupy tetrahedral (Td) and octahedral (Oh) positions respectively. In order to understand the behaviour of nanoparticles of these metal ferrites for the photocatalytic water splitting reaction, we use a combination of computational simulations and experimental data to investigate the bulk and the surfaces properties of MFe2O4 (A =Co, Cu or Zn).

The A and B cations can redistribute across the Td and Oh sites and our results showed that the Td/Oh ratio of the Fe cation on the bulk was different from the surface. Calculations show that the electronic structure and band gap is affected by the cation distribution which in turn influences the catalytic properties. Bulk characterization was done by Anomalous X-Ray scattering, X-Ray Diffraction and XANES while the surface characterization was carried out by X-ray magnetic Circular Dichroism and Near Edge X-Ray Absorption Fine Structure (NEXAFS).

STM of ultrathin MnxNbyOz nanophases on Au(111)

Ge T[1], Castell M[1]
[1]Department of Materials, University of Oxford

Metal-supported two-dimensional (2D) metal oxides are a scientifically intriguing and technologically significant class of materials. Their reduced dimensionality, combined with interactions between the oxide and the support, gives rise to novel oxide phases, many of which have no bulk equivalents. Compared to binary systems, 2D ternary oxides have compositional flexibility that can add new degrees of freedom resulting in complex crystal structures. These have the potential for novel applications due to their unique electronic and optical properties(1).

Here we report successful on-surface synthesis of MnxNbyOz phases on the Au(111) surface. The growth evolution and structure of nanostructures and thin films are investigated by Scanning Tunnelling Microscopy (STM). The ternary oxides are grown by either co-deposition and oxidation of Mn and Nb, or using a well investigated binary phase (a Nb2O3 monolayer or a MnOx fishbone phase) as a template(2,3). By adjusting the reacting conditions of the deposits, formation of distinctly different phases with various Mn / Nb ratios can be achieved. The diversity of Au(111) supported MnxNbyOz nanostructures and films demonstrates the potential to tune surface functionality by adjusting the oxide stoichiometry.

1. Netzer et al., Oxide thin films and nanostructures. Oxford University Press: 2021.
2. Wang et al., Phys. Rev. B 2019, 100, 125408.
3. Chen et al., Surf. Sci. 2023, 730, 122248.

Liquid Brain, Excitable Liquid Interfaces as Computational Substrates for Molecular Characterization

Hermans R[1], Shrivastava S[1], Shrivastava A[1], Thomas A[1], Caramazza P, Meghdadi A[1], Bailey J, St John A[1], Lam E[1], Lee S[1]
[1]Apoha Limited

Understanding and harnessing the physical properties of interfaces is critical for advancing both fundamental science and applied technologies. We introduce the Liquid Brain®, a biomimetic, excitable liquid interface that enables real-time, high-dimensional state diagram embeddings of molecular and colloidal systems. This approach exploits surface wave dynamics and out-of-equilibrium thermodynamics to extract multi-parameter biophysical insights from minimal sample volumes. Using as little as 10 µg of material, the system generates single-shot classifications of complex biological molecules, enabling predictive assessment of antibody developability and formulation stability.

Our novel approach uses mechanically excitable lipid and liquid interfaces as computational substrates, where wave propagation encodes molecular interactions at the interface. Recent studies benchmarked over 100 clinical-stage antibodies, revealing developability insights beyond conventional screening methods. Beyond pharma, the technology promises broad applicability across protein formulations, lipid interactions, and material discovery, bridging fundamental surface science with industrial applications.

These findings establish a new paradigm for surface-driven biophysical analysis, leveraging integrated multi-dimensional interfacial dynamics as a platform for high-throughput molecular characterization. The Liquid Brain® exemplifies how excitable interfaces can serve as neuromorphic wetware, offering a scalable and physically grounded approach to answer material questions using physical reservoir computing.

Sliding of a liquid spherical droplet in an external insoluble liquid at low Reynolds numbers

Lebedev-stepanov P[1]
[1]Shubnikov Institute of Crystallography, Kurchatov Complex of Crystallography and Photonics

The experiment shows that small liquid droplets under the action of gravity and the Archimedes force move in the external viscous liquid practically according to the Stokes drag force equation, and not in accordance with the Hadamard–Rybczynski (HR) formula, which was specially developed to describe the motion of a liquid droplet in an external viscous liquid.

Various mechanisms are proposed to explain this: increased viscosity at the interface between two liquids and the presence of unaccounted surfactants. However, there is another fundamental mechanism that has not been taken into account. It can be expected that the velocities of such liquids, insoluble in each other, may not equalize at the boundary of the droplet. No slip condition may be may be unnatural at the droplet interface. In this paper, the Navier condition is applied to the liquid-liquid boundary for the first time.

A generalized HR equation is obtained. If slip length $\lambda=0$ that equation transforms into the usual HR equation. At certain λ, we arrive at a model with continuity of the components of the viscous stress tensor at the interface of two fluids. For infinite viscosity of the drop, it becomes a well-known relation generalizing the Stokes drag force for a solid sphere, taking into account the boundary condition of partial slip [1].

[1] P. Lebedev-Stepanov. ArXiv:2502.02814v2 [physics.flu-dyn]

O_2 Dissociation on α-Fe_2O_3(1$\bar{1}$02)-(1×1)

Lewis F[1], Rafsanjani-Abbasi A[1], Buchner F[1], Conti A[1], Kraushofer F[1], Sombut P[1], Eder M[1], Pavelec J[1], Rheinfrank E[1], Franceschi G[1], Birschitzky V[2], Riva M[1], Franchini C[2], Schmid M[1], Diebold U[1], Meier M[2], Madsen G[1], Parkinson G[1]
[1]TU Wien, [2]University of Vienna, [3]Universita di Bologna

Single-atom catalysis (SAC) is a rapidly growing field of research motivated by the desire to decrease the amount of precious metals used for facilitating catalytic reactions. Similar to homogeneous catalysis, SACs also lead to well defined single-atom centers required for selectivity. However, for reactions like molecular O2 dissociation, two active sites in close proximity are generally needed. In this poster, we will be examining the question: Can the diatomic molecule O2 dissociate at a single Pt atom on a well-defined hematite surface, α-Fe2O3(1$\bar{1}$02)-(1×1)?

Scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and density functional theory (DFT) have recently been used to characterize Pt single atoms on hematite [1]. Here, we have intentionally oxidized Pt SAC by annealing in an O_2 background and studied the surface using non-contact atomic force microscopy (nc-AFM) with a well-defined copper oxide (CuOx) tip [2]. The images show an attractive species, the Pt adatoms, and two repulsive features, presumably the dissociated oxygen atoms. Additionally, the Pt^{2}+ component increases in the XPS measurements, indicating an oxidation of the Pt atoms. Computational studies aimed at understanding the structure of these species are in progress.

1. Rafsanjani-Abbasi, A., et. al. Digging Its Own Site: Linear Coordination Stabilizes a Pt1/Fe2O3 Single-Atom Catalyst, ACS Nano, 2024. 39, 26920.
2. Lammers, B. S., et. al, Benchmarking atomically defined AFM tips for chemical-selective imaging. Nanoscale, 2021, 13, 13617.

Squeezing of Adsorbates in the Caldeira Leggett Model

Ord M[1]
[1]University Of Cambridge

As the quantum analogue of the Langevin equation, the Caldeira Leggett Model describes the diffusion of a quantum system connected to an environment [1]. While formally exact, the method is computationally expensive. To choose the correct technique, it is therefore necessary for us to identify which systems see a significant quantum effect.

In the Caldeira Leggett Model, the system density matrix can first be separated into a series of realizations, each governed by the stochastic Schrödinger equation. In this paper, we study the dynamics of the squeezed coherent states [3] within this framework. We show that a harmonic system initially prepared in such a state remains so for the entire simulation, and derive a new formula for their evolution. Crucially, we find that the dynamics of squeezing is entirely deterministic, and we can therefore derive an explicit formula for the pairwise uncertainty relation. By applying this formula to a series of previously studied systems [2], we show that we can accurately identify the quantum-to-classical transition.

[1] Breuer, H.-P. & Petruccione, F. The Theory of Open Quantum Systems.
[2] Torres-Miyares, E. E. et al. The stochastic wave function method for diffusion of alkali atoms on metallic surfaces. Phys. Chem. Chem. Phys. 25, 6225–6231 (2023).
[3] Gerry, C. & Knight, P. Introductory Quantum Optics. (Cambridge University Press, Cambridge, 2004). doi:10.1017/CBO9780511791239.

A first principles study on 2 dimensional Zinc Carbide

Sengupta A[1,2]
[1]P.d. Women's College, [2]University of North Bengal

In this work, with density functional theory calculations we study two-dimensional ZnC. For its structural, electronic, and optical properties. From the DFT calculations employing the generalized gradient approximation (GGA) with the Perdew Burke Ernzerhoff (PBE) exchange and correlation functional, we find out the various properties of this novel material. The structural optimizations show 2D ZnC to stabilize in the two-dimensional planar hexagonal structure with a lattice parameter of 3.28Å, with Zn-C bond length of 1.95Å. The 2D material showed a zero-gap bandstructure suggesting a metallic nature. Charge density and electron localization function (ELF) studies show a rather de- localized charge distribution and electron gas like features in between. The optical properties calculated with the random phase approximation (RPA) show a strong absorption peak at 109nm with significant absorption lines present at 88 and 190nm.

Circular dichroism study of alanine on Cu(110) as a model for enantioselective heterogeneous catalysis

Karagoz B[1], Teather E[2], Held G[1]
[1]Diamond Light Source, Harwell Science and Innovation Campus, [2]Department of Physics, University College London

Many pharmaceutical applications require a specific chiral enantiomer, so developing enantioselective production methods is important. Heterogeneous catalysis is relatively inexpensive, but metal surfaces are achiral, so produce racemic mixtures. However, chirality may be imparted through adsorption of so-called chiral modifiers. Alanine on Cu(110) is a well-studied, simple model for this process, in which the alanine layers form chiral and achiral superstructures after deposition and annealing [1,2]. We seek to better understand the interactions between alanine and Cu.

In our recent measurements at FiNEstBeAMS at MAX-IV laboratories, we probed the valence band of D- and L-alanine on Cu(110) by x-ray circular dichroism (CD) photoemission and absorption. It has previously been shown that the enantiomers show a large, opposite CD signal in the low x-ray range [3]. We observed this effect persists when alanine is adsorbed on Cu(110), but it was lost when the superstructure transformed to achiral. This has implications for the nature of the superstructures and bonding at the surface.

[1] S. M. Barlow et al., Surface Science, 590(2), 243–263, 2005;
[2] B. S. Mhatre et al., Chemical Communications, 52(98), 14125–14128, 2016;
[3] U. J. Meierhenrich et al., Angewandte Chemie International Edition, 49(42), 7799–7802, 2010;

The adsorption height of nitrogen doped graphene grown by chemical vapour deposition

Thompson A[1,2], Stoodley M[2,3], Straw J[1], Clarke M[1], Warwick L[1], Eratam F[2], Williams L[2,4,5], Klein B[2,3], Goto F[2,6], Lee T[2], Saywell A[1], Maurer R[3,7], Duncan D[1,8]
[1]University of Nottingham, [2]Diamond Light Source , [3]Department of Chemistry, University of Warwick, [4]School of Physics and Astronomy, University of Glasgow, [5]School of Chemistry, University of Glasgow, [6]Department of Physics, Politecnico di Milano, [7]Department of Physics, University of Warwick, [8]School of Chemistry, University of Nottingham

The remarkable electronic, mechanical and thermal properties of graphene make it one of the most promising two-dimensional materials [1]. The intentional introduction of functional defects into graphene via nitrogen doping is a promising route for customising the chemical, electronic and catalytic properties of graphene [2]. Understanding the interaction of these N-dopants with their growth substrate is important for characterising how these defects are grown into the graphene lattice and to understand how these defects interact with the world around them. A primary indicator of the interaction between an adsorbate and the substrate is its adsorption structure as it indicates the strength of interaction between the two. Herein, we have used X-ray standing waves (XSW) [3] to determine the structure of the N-dopants in graphene in a chemically resolved manner from films grown via ultra-high vacuum chemical vapour deposition of molecular precursors, azabenzopyrene and phthalocyanine on a Cu(111) surface as a function of substrate growth-temperature.

References:

[1] A. Geim, K. Novoselov, Nature Mater ,2007, 6, 183–191
[2] Y. Shao, S. Zhang, M. H. Engelhard, et al, J. Mater. Chem, 2010, 20(35), 7491–7496.
[3] D. P. Woodruff, Rep. Prog. Phys., 2005, 68(4), 743.

Synthesis and Characterization of Single-Layer Two-Dimensional M2(HITP)3 {M= Ni, Fe} Metal-Organic Frameworks on Au(111)

Tyagi S[1], Shu S[1], Forssberg A[1], Patrick C[1], Castell M[1]
[1]Department of Materials, University of Oxford

Two-dimensional Metal-Organic Frameworks (2D-MOFs) are networks composed of metallic nodes connected by conjugated organic molecules [1]. 2D MOFs have attracted significant attention because of their sufficiently high electrical conductivity for use in applications like chemiresistive sensing and as electrocatalysts [2].

Theoretical predictions suggest that 2D-MOFs composed of transition metal centres and triphenylene derivative molecules can behave as topological insulators and exhibit the quantum anomalous Hall effect [3, 4]. However, experimental realization of these interesting non-trivial properties remains challenging. This happens because conventional wet chemical synthesis of MOFs produces multi-layered structures due to interlayer interactions, whereas these properties are being predicted for single-layer structures. To bridge this gap, synthesis of single-layer 2D MOFs is desirable.

Here, we report the synthesis of single-layer two-dimensional Ni-hexaiminetriphenylene {Ni3(HITP)2} and Fe-hexaiminetriphenylene {Fe3(HITP)2} MOFs on Au(111) surface. Using Scanning Tunnelling Microscopy (STM), we studied the growth and formation of these MOFs. STM imaging enables us to visualize individual molecules and metal centres within the MOFs, offering a detailed view of their structures [5]. This level of characterization is crucial for addressing fundamental questions about the structure-property relationships in these materials. Our interpretations of the STM images are further supported by density functional theory (DFT) calculations.

1. Wang et al. Chem. Soc. Rev., 2021, 50, 2764-2793.
2. Michael Ko et al. Chem. Commun., 2018, 54, 7873-7891.
3. Wang et al. Nano Lett. 2013, 13, 2842–2845.
4. Wang et al. Phys. Rev. Lett. 2013, 110, 196801-196806.
5. Fubiao Gu et al. J. Phys. Chem. C 2024, 128, 17797−17805.

Tuning 2D perovskite for photocatalysis

Zhang H[1], Tsang S[1]
[1]Univ. Of Oxford

Photocatalytic decomposition of NH_3 with reducing heat is essential for decreasing H_2 production costs. However, efficient photocatalysts for NH_3 decomposition are scarce, hindering the further application of this technology. Herein, we present a hydrazine-intercalated layered perovskite, $(N_2H_4)_{0.5}PrNb_2O_7H$, which exhibits the highest NH_3 decomposition rate compared with all photocatalysts reported in literature.

This study is also the first to report this unique property of perovskite oxides, wherein N_2H_4 molecules can be stabilised at the interlayer space. Through a series of characterisation, including Neutron Powder Diffraction, in-situ Synchrotron XRD, in-situ PDF and in-situ XAS, we confirmed the position, occupancy and formation process of N_2H_4 molecules within the perovskite interlayer gallery. With the progressive increase of temperature during photocatalysis, the H_2 evolution rate could reach to ~2.3 mmol/gh at 200 °C, highlighting the synergistic effect of thermal and photo contributions to NH_3 decomposition.

Hence, this finding highlights the potential of 2D layered perovskite in advancing NH_3 decomposition technology, which provides valuable insights for the design and optimisation of 2D perovskite photocatalysts for various catalytic applications.