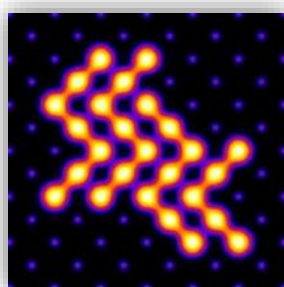

SURFACE SCIENCE DAY

11th December 2017

ABSTRACT BOOK



UNIVERSITY OF
LIVERPOOL



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SPECSTM

Welcome to Surface Science Day @ University of Liverpool 2017!

We are pleased to welcome you to the latest in this series of one-day conferences. The inaugural conference was held at the University of Central Lancashire in 2015 and was a great success, though we have even more registrations this time round, with 82 registered participants from 22 different institutes!

The event is intended to be an opportunity for new students and postdocs to hear about the latest in surface science research from leaders in the field, with plenty of time allocated for meeting others in the community over tea and coffee and an extended lunch and poster presentation.

It is a great opportunity for young scientists to establish networks with research leaders, allowing for the transfer of knowledge and generation of lasting collaborations and friendships.

We are able to keep the meeting free thanks to donations from sponsors. These sponsors also contribute towards the Poster Prize, which will be awarded at the end of the day. We also gratefully acknowledge the Surface Science Research Centre at the University of Liverpool for further support for the conference.

Thanks for supporting this event and we look forward to welcoming you to future events in the series!

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SSD Committee.

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General Information

Venue:

Surface Science Day 2017 will take place in the Leggate Theatre of the Victoria Gallery & Museum (maps and directions to the building are provided overleaf). The Leggate theatre is located on the second floor of the building, where there will also be a registration desk. Signage will be provided on the day.



Refreshments and Lunch:

Tea and coffee breaks, lunch, and evening refreshments will be served in the neighbouring room to the lecture theatre. There is plenty of space in the theatre itself and surrounding halls to eat, drink and network.

Poster Presentation:

Poster presentations will take place at the back of the lecture theatre over lunch. For those presenting a poster, you can hang your poster during the welcome or the coffee break pre-lunch. The best student poster will be awarded a certificate and cash prize.

Photo:

A group photo will be taken in the meeting hall after lunch.

Contact:

If you have any problems regarding directions, travel or any other general queries contact Sam Coates on 07972043308.

Programme

09:00	Coffee, registration		
09:30	Welcome	Rasmita Raval, Director of SSRC	University of Liverpool
09:35	Tautomerization in single Porphycene molecules on metal surfaces	Mats Persson	University of Liverpool
10:10	Functionalising metal surfaces	Christopher Baddeley	University of St Andrews
10:45	Coffee		
11:15	Lone pair states at the surfaces of oxides of the post transition metals	Russ Egdell	University of Oxford
11:50	Recent advances in the high-resolution characterization of functional macro molecules at surfaces	Giovanni Costantini	University of Warwick
12:25	Physical and chemical aspects of surface chirality	Stephen John Jenkins	University of Cambridge
13:00	Lunch and poster session		
14:45	Self-organised (C60) _m -(Au) _n magic number clusters- Specific configurations from non-specific interactions	Quanmin Guo	University of Birmingham
15:20	Exploring complexity in surface supramolecular arrays	Neil Champness	University of Nottingham
15:55	Surface science dynamics on the femtosecond time scale at Central Laser Facility	Cephise Cacho	STFC Rutherford Appleton Laboratory
16:30	Coffee		
17:00	Using surface science techniques to understand the formation of stars and planets	Wendy Brown	University of Sussex
17:35	Understanding oilfield corrosion: a surface science approach	Rob Lindsay	University of Manchester
18:10	Poster prize and closing	Ronan McGrath, Head of School of Physical Sciences	University of Liverpool
18:15	Refreshments		

List of Posters

No.	Poster Title	Name	Affiliation
P1	Correlation of the optical and nanomechanical properties of C ₆₀ -2DM heterostructures fabricated by a hybrid electrospray and Langmuir-Blodgett technique	Angelo Lamantia	Lancaster University
P2	Smart Switchable Biological Surfaces for On-demand Biosensing	Bárbara Simões	University of Birmingham
P3	Spin and Angle-Resolved PES of Si(110)“16x2” surfaces	Elaine Seddon	University of Manchester
P4	Supramolecular Surfaces for Protein Immobilisation	Giuseppe Di Palma	University of Birmingham
P5	Surface Enhanced Raman spectroscopy of a molecular sensor for hydrogen bonding and metallization	Heike Arnolds	University of Liverpool
P6	Self-Assembly and On-Surface Reactions of Binol Molecules on Copper Surfaces	James Lawrence	University of Warwick
P7	High intensity electrospray source for UHV deposition of large functional molecules for in-situ STM studies	Luis M.A. Perdigo	University of Warwick
P8	Imaging subsurface defects in WS ₂ /WSe ₂ CVD flakes via Ultrasonic Force Microscopies	Marta Mucientes	Lancaster University
P9	Characterising inhibited interfaces using Vibrational Sum-Frequency Spectroscopy	Michael Jennifer Grace Dowhyj	University of Manchester
P10	Nile red self-assembly on Au(111) surface	Oreste De Luca and Marco Turano	Università della Calabria
P11	Epitaxial Growth of Monolayer MoS ₂ on SrTiO ₃ Single Crystal Substrates	Peiyu Chen	University of Oxford
P12	Two-Dimensional Electron Gases on the CdO Surface	Pip Clark	University of Manchester
P13	Fibonacci modulation of a C ₆₀ thin film	Sam Coates	University of Liverpool
P14	Molecules within molecules: a NIXSW study of H ₂ O@C ₆₀	Sam Jarvis	Lancaster University
P15	Nucleation, Growth and Aggregation of NbO _x Clusters on Au(111) Surfaces	Shuqiu Wang	University of Oxford
P16	Preparation of benzoboroxole-modified gold surfaces for selective glycoprotein recognition	Yazmin Kaur Tagger	University of Birmingham
P17	An investigation of double molecular layers of C ₆₀ /C ₇₀ and C ₇₀ /C ₇₀	Yitao Wang	University of Birmingham
P18	Reversible CO ₂ absorption with a superbasic ionic liquid: A near-ambient pressure X-ray photoelectron spectroscopy study	Zoë Henderson	University of Central Lancashire
P19	Strategies for molecular imprinting of prostate cancer biomarkers on Au substrates – adapting surface chemistry to clinical diagnostics	Joshua Norman	University of Birmingham

9:35am

Tautomerization in Single Porphycene Molecules on Metal Surfaces

Mats Persson¹,

¹*University of Liverpool*

We have investigated tautomerization in single porphycene molecules on metal surfaces by a combination of low-temperature scanning tunneling microscopy (STM) experiments and density functional theory (DFT) calculations [1-5]. We show that this tautomerization on the Cu(110) surface can be precisely controlled by placing, with atomic precision, a copper adatom close to a porphycene molecule [2]. The tautomerization can also be induced by the force from a tip [3]. Force spectroscopy quantifies the force needed to trigger tautomerization with submolecular spatial resolution. Our DFT calculations show how the reaction pathway and barrier of tautomerization are modified in the presence of a copper tip and reveal the atomistic origin of the process. On the Ag(110) surface, we show that the double hydrogen atom transfer proceed by tunneling [4]. The observed kinetic isotope effect for three isotopologues and DFT calculations indicate that a stepwise transfer mechanism is dominant. The tautomerization rate can also increase by vibrational excitation via an inelastic electron tunneling process. On the (111) surfaces of Cu, Ag and Au, the mismatch of the symmetry of the porphycene molecule and the (111) surface results in a more complex behaviour of the potential energy surface and the tautomerization [5].

[1] *Thermally- and vibrationally-induced tautomerization of single porphycene molecules on a Cu(110) surface*, T. Kumagai, F. Hanke, S. Gawinkowski, J.C. Sharp, K. Kotsis, J. Waluk, M. Persson, and L. Grill, *Physical Review Letters* **111**, 246101 (2013)

[2] *Controlling intramolecular hydrogen transfer in a porphycene molecule with single atoms or molecules located nearby*, T. Kumagai, F. Hanke, S. Gawinkowski, J. Sharp, K. Kotsis, J. Waluk, M. Persson, and L. Grill, *Nature Chemistry* **6**, 41 (2014)

[3] *Force-induced tautomerization in a single molecule*, J. N. Ladenthin, T. Frederiksen, M. Persson, J. C. Sharp, S. Gawinkowski, J. Waluk and T. Kumagai, *Nature Chemistry* **8**, 935 (2016)

[4] *Direct observation of double hydrogen transfer via quantum tunneling in a single porphycene molecule on a Ag(110) surface*, M. Koch, M. Pagan, M. Persson, S. Gawinkowski, J. Waluk, and T. Kumagai, *Journal of American Chemical Society* **139**, 12681 (2017)

[5] *Quantum Tunneling in Real Space: Tautomerization of Single Porphycene Molecules on the (111) Surface of Cu, Ag, and Au*, T. Kumagai, J. Ladenthin, Y. Litman, M. Rossi, L. Grill, S. Gawinkowski, J. Waluk and M. Persson (submitted to *Journal of Chemical Physics*)

10:10am

Functionalising metal surfaces

Christopher J Baddeley¹

¹*EaStCHEM School of Chemistry, University of St Andrews, North Haugh, St Andrews, Fife, KY16 9ST, UK*

Metal particles modified by the adsorption of chiral molecules (modifiers) have been successfully used as heterogeneous catalysts for enantioselective hydrogenation reactions.[1, 2] Crucial to the success of such catalysts are hydrogen-bonding interactions between the adsorbed chiral modifier and the pro-chiral reagent which control the geometry of the reactant favouring the surface catalyzed hydrogenation to one enantiomeric product. Catalytic selectivity is limited by a number of factors; most notably: the diversity of active sites available on the surface of a metal particle and the loss of chiral modifiers under catalytic conditions. Our work aims to construct thermally stable, chiral architectures on catalytically active surfaces with the target of forming uniform arrays of chiral docking sites to optimize catalytic enantioselectivity. Supramolecular self-assembly at surfaces to form porous H-bonded networks,[3] metal-organic coordination networks [4] or covalent architectures [5] is an important means of controlling host-guest interactions. Much work on supramolecular self-assembly has exploited weak adsorbate-metal interactions and control over intermolecular interactions to facilitate construction of well-defined 2-D architectures. On more reactive metal surfaces such as Ni, Pd or Pt, the strong chemical interaction between functional groups and the metal surfaces can lead to reorientation and/or decomposition of the adsorbate, hence restricting the ability to produce high quality 2-D frameworks on these, more catalytically interesting, metals.[6] We outline strategies for the formation of chiral metal-organic architectures on metal surfaces [7] and protocols to prepare porous covalent-organic frameworks on reactive metal surfaces.[8]

[1] Y. Izumi, *Advances in Catalysis*, **32**, 215 (1983).

[2] T. Mallat, E. Orglmeister, A. Baiker, *Chemical Reviews*, **107**, 4863 (2007).

[3] J.A. Theobald, N.S. Oxtoby, M.A. Phillips, N.R. Champness, P.H. Beton, *Nature*, **424**, 1029 (2003).

[4] L. Bartels, *Nature Chemistry*, **2**, 87 (2010).

[5] M. Lackinger, *Polymer International*, **64**, 1073 (2015).

[6] J. Greenwood, H.A. Früchtl, C.J. Baddeley, *J. Phys. Chem. C*, **116**, 6685 (2012).

[7] R.T. Seljamäe-Green, G.J. Simpson, F. Grillo, J. Greenwood, S.M. Francis, R. Schaub, J.E. Gano, H.A. Früchtl, P. Lacovig, C.J. Baddeley, *Langmuir*, **31** (2015) 262.

[8] C.R. Larrea, C.J. Baddeley, *Chemphyschem*, **17** (2016) 971.

11:15am

Electron lone pairs at oxide surfaces

Russell G Egdell¹

¹*Department of Chemistry, University of Oxford, Inorganic Chemistry Laboratory, University of Oxford OX1 3QR
(russell.egdell@chem.ox.ac.uk)*

Post transition elements such as Sn and In have two main oxidation states: the group (N) oxidation state (N=4 for Sn and N=3 for In) and the so-called N-2 state where formally the metal has a $5s^2$ valence electron configuration. Localised and stereochemically active lone pairs develop when post transition metals in the N-2 oxidation state occupy crystallographic sites lacking inversion symmetry. The lone pairs arise from hybridisation between anion states and occupied metal s states to give antibonding states close to the top of the valence band, which hybridise further with nominally empty metal p states. This mixing is only possible in non-centrosymmetric sites because s and p states are of opposite parity [1].

There has been speculation over many years that lone pairs should develop at the surfaces of compounds of post transition metal compounds because surface sites of necessity lack inversion symmetry. There have been many reports of electronic states toward the bottom of the bulk bandgap in photoemission spectra of materials such as Ga_2O_3 , In_2O_3 and SnO_2 , but the unambiguous identification of a surface lone pair surface state has proved elusive. In the present contribution we show that by comparing hard and soft X-ray photoemission spectra of vacuum-annealed $In_2O_3(111)$ ($1\times$) it becomes obvious that a gap state seen previously and assigned to bulk oxygen vacancies[2] is in fact localised at the crystal surface. Re-analysis of previously published LEED I/V data [3] and correlation with STM images reveals that the vacuum annealed surface contains an ordered array of indium adatoms. DFT calculations show that these adatoms act as three electron donors. Each adatom traps two electrons in a lone pair surface state, while the third electron is delocalized into a two dimensional electron gas, giving a surface electron accumulation layer [4].

[1] A Walsh, D J Payne, R G Egdell and G W Watson, Chemical Society Reviews 2011 **40** 4455 – 4463

[2] K H L Zhang, R G Egdell, F Offi, S Iacobucci, L Petaccia, S Gorovikov and P D C King
Physical Review Letters 2013 **110** 056803/1-5

[3] K Pussi, A Matilainen, V R Dhanak, A Walsh, R G Egdell and K H L Zhang, Surface Science 2012 **606** 1-6

[4] P D C King, T D Veal, D J Payne, A Bourlange, R G Egdell and C F McConville, Physical Review Letters 2008 **101** 116808/1-4

11:50am

Recent advances in the high-resolution characterization of functional macro molecules at surfaces

Giovanni Costantini¹

¹Department of Chemistry, University of Warwick, Gibbet Hill Rd, CV4 7AL, Coventry, UK

Understanding the interaction between functional macromolecules and inorganic surfaces lies at the heart of a number of fundamental and industrial research areas with applications ranging from healthcare to energy, from food to environmental protection. In particular, the ability to characterise the resulting interfaces at high spatial resolution has been the key to significant advancements in the field and is thus a major investigation topic.

This talk will present recent advances in the use of high-resolution scanning tunneling microscopy (STM) to analyse a number of molecule-surface model systems with increasing complexity. It will start by discussing the limits that standard molecular deposition techniques impose on the size of molecular units that can be studied in surface science. It will then move to demonstrate that these limitations can be overcome by using soft ionisation techniques capable to transfer thermolabile complex molecules in the gas phase and to soft land them intact onto surfaces under fully controlled deposition conditions. In particular, it will be shown that a combination of electrospray vacuum deposition and high-resolution STM allows the imaging of individual macromolecules with unprecedented detail, thereby unravelling structural and self-assembly characteristics that have so far been impossible to determine.

The case of conjugated polymers will be investigated in details, showing that sub-monomeric resolution STM images allow us to precisely sequence a complex co-polymer by simply counting its repeat units. More importantly, it will be demonstrated that it is possible to identify, precisely determine the nature, locate the position, and ascertain the number of defects in the polymer backbone. This unique insight into the structure of a polymer is not attainable by any other existing technique and solves a crucial challenge in polymer analytics.

12:25pm

Physical and Chemical Aspects of Surface Chirality

Stephen John Jenkins¹

¹*University of Cambridge*

Over the past two decades, a great deal of progress has been made towards an understanding of the various ways in which chirality at surfaces can influence the chemistry that takes place on them.

A key theme has been the propagation of asymmetry from the length-scale of a single molecule, through that of the molecule's local environment, up to that of an extended supra-molecular network. Rather less attention has been paid to the physics of chiral surfaces, despite the fact that mechanical, optical, magnetic and electronic aspects of the surface are all likely to be influenced by structural asymmetry.

This talk aims not only to provide an overview of achievements in chiral surface physics and chemistry, but also to point towards the challenges and opportunities associated with bringing these two fields together.

14:45pm

Self-organised $(C_{60})_m-(Au)_n$ magic number clusters- Specific configurations from non-specific interactions

Quanmin Guo¹

¹*School of Physics and Astronomy, University of Birmingham, Birmingham, B15 2TT, UK*

In order to explore the possibility for designing and fabricating nanostructures based on non-directional bonding, we have recently investigated a Fullerene-metal coordinated system and produced magic number, hybrid $(C_{60})_m-Au_n$ clusters on the Au(111) surface. The smallest magic number cluster, $(C_{60})_7-Au_{19}$, consists of a hexagonal 19 Au atom island capped by seven C_{60} molecules. One of the molecules sits directly above the gold island, the remaining six molecules sit next to the edges of the gold hexagonal island. Other magic number clusters such as $(C_{60})_{10}-Au_{35}$ and $(C_{60})_{12}-Au_{49}$ have also been produced. Take the $(C_{60})_7-Au_{19}$ cluster for example, the molecule-molecule vdW bonding is optimized by maintaining a $C_{60}-C_{60}$ distance very close to the distance in bulk C_{60} . Molecule-Au bonding is also optimized by attaching each of the surrounding six molecules to a step edge. The higher charge density at the step edge favours the charge transfer from Au to C_{60} . The result is that this $(C_{60})_7-Au_{19}$ cluster has a remarkable stability. The 19-Au island on its own is not stable beyond 200 K, a $(C_{60})_7$ cluster on its own is not stable beyond 240 K. The hybrid cluster, however, is stable up to 400 K. The hybrid clusters are held together by neither directional H-bonding nor covalently bonding. Instead, the collective interaction among all the constituents within the cluster is responsible for the stability of the cluster. We call this type of metal-organic coordination “globally optimized metalorganic coordination”.

[1] Xie, Y-C; Tang, L.; Guo, Q. “Cooperative assembly of magic number C_{60} -Au complexes”. *Phys. Rev. Lett.* 111 (2013) 186101.

[2] Kaya, D.; Bao, D-L.; Palmer, R. E.; Du, S-X.; Guo Q. “Tip-triggered thermal cascade manipulation of magic number gold-fulleren clusters in the scanning tunnelling microscope” *NANO Lett.* 17 (2017) 6171-6176.

15:20pm

Exploring Complexity in Surface Supramolecular Arrays

Neil R. Champness¹

¹*School of Chemistry, University of Nottingham, Nottingham, NG7 2RD, UK*

Non-covalent directional intermolecular interactions provide a recognition pathway which has been widely exploited in supramolecular chemistry to form functional nanostructures in both solution and in the solid-state. Our studies using hydrogen-bonding interactions to enable the directed assembly of extended nanostructures will be presented and in particular the lecture will focus on our work investigating surface-based self-assembly processes and the creation of complex structures.¹ The talk will include studies that demonstrate unprecedented control of supramolecular topology (Fig. i)² the first direct observation of a molecular-scale glass (Fig. ii)³ and the generation of a new class of porphyrin molecular tiles that are functionalised with DNA bases.⁴ Recent developments in scanning probe microscopy allow direct visualisation of sub-molecular features (Fig. iii).⁵ Most importantly our work establishes a direct connection between crystal engineering, supramolecular chemistry and nanostructure fabrication.

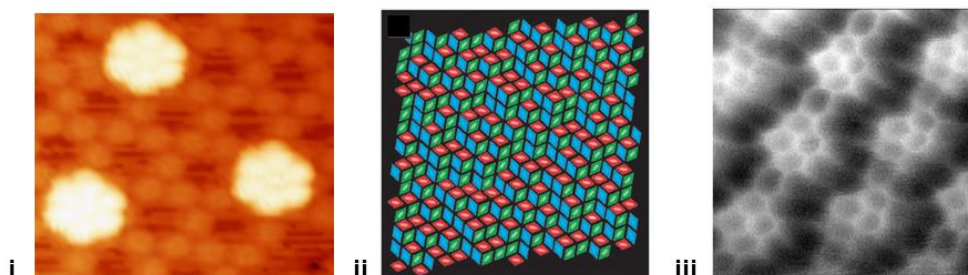


Figure: **i** STM image of a surface supramolecular framework hosting heptamers of C_{60} molecules;¹ **ii** random rhombus tiling demonstrated using tetracarboxylic acid molecules;² **iii** DFM image of a hydrogen-bonded array with sub-molecular detail.⁴

[1] C.R. Pfeiffer, N. Pearce, N.R. Champness, *Chem. Commun.*, 53, 11528 (2017).

[2] J.A. Theobald, N.S. Oxtoby, M.A. Phillips, N.R. Champness, P.H. Beton, *Nature*, **424**, 1029 (2003).

[3] M.O. Blunt, J. Russell, M.C. Giménez-López, J.P. Garrahan, X. Lin, M. Schröder, N.R. Champness, P.H. Beton, *Science*, **322**, 1077 (2008).

[4] A.G. Slater, Y. Hu, L. Yang, S.P. Argent, W. Lewis, M.O. Blunt, N.R. Champness, *Chem. Sci.*, **6**, 1562 (2015).

[5] A. M. Sweetman, S. Jarvis, H. Sang, I. Lekkas, P. Rahe, Y. Wang, J. Wang, N.R. Champness, L. Kantorovich, P.J. Moriarty, *Nature Commun.*, **5**, 3931 (2014).

15:55pm

Surface Science Dynamics on the Femtosecond Time Scale at Central Laser Facility

Dr. Céphise Cacho¹

¹Artemis Central Laser Facility, Rutherford Appleton Laboratory, United Kingdom

The Central Laser Facility is a UK national laboratory operating five user facilities based on state-of-the-art laser sources. Amongst them Ultra and Artemis are offering ultrafast time resolved spectroscopy techniques to investigate surface dynamics on various systems. In this talk I will present a recent result on the role of Mo(bypy)(CO)₄-electrode interactions during CO₂ reduction. Using the Sum Frequency Generation technique, it is possible to explore the different vibrational mode of the Mo molecules at the electrode interface.

The Artemis facility is specialised in High Harmonic Generation in gas to produce ultrashort XUV pulses that are mainly used for time resolved electron spectroscopy. Using ARPES technique I will show how we can investigate the electron dynamics at the surface of novel quantum materials such as graphene and transition metal dichalcogenides (TMDC). Finally a joint development of the facilities (Ultra and Artemis) involving new laser technology at high repetition rate will be presented with the perspective of new scientific capabilities.

17:00pm

Using surface science techniques to understand the formation of stars and planets

Wendy Brown¹

¹*Chemistry, University of Sussex, Falmer, Brighton, BN1 9QJ.*

Over 180 molecules have now been conclusively identified in various regions of space. Many of these molecules are present in abundances that indicate that they cannot be made in the gas phase. Astronomers have speculated that surface chemistry, taking place on dust grains, is responsible for the formation of many of the molecules found in space, including in star forming regions. Dust grains are carbonaceous and siliceous in nature and are often covered in films of molecular ices at the low temperatures (20-30 K) of space. These molecular ices are formed of around 60-70% water ice, but also contain large amounts of methanol, carbon dioxide and ammonia, along with a number of so-called complex organic molecules (COMs).

With this in mind, we have undertaken detailed surface science investigations of a family of COMs with the chemical formula $C_2O_2H_4$ (namely methyl formate, glycolaldehyde and acetic acid) on a graphitic dust grain analogue surface. Temperature programmed desorption (TPD) and reflection absorption infrared spectroscopy (RAIRS) are used to investigate the adsorption and thermal and ultra-violet processing of ices containing these COMs and water ice in conditions that simulate star forming regions. We also use our data to model the desorption of the molecular ices from grain surfaces under conditions relevant to space. This information can be used by astronomers to model the formation of stars and planets.

17:35pm

Understanding Oilfield Corrosion: A Surface Science Approach

R. Lindsay¹

¹*University of Manchester*

Material degradation resulting from corrosion is an omnipresent concern. Not only is there a huge economic cost, estimated to be ~ €2 trillion per annum globally, but it can also lead to destruction of the environment, as well as the loss of life. Given this importance, there is a large ongoing effort to understand and control corrosion, with both academic and industry based researchers active in this area. Significant advances have been achieved, including the development of innovative corrosion control solutions. Atomic scale, mechanistic insight into pertinent phenomena, however, often remains elusive, hindering further progress. Such work is clearly the domain of the surface scientist, but it has not proven to be the most fashionable topic to date.

In this talk, our recent efforts to begin to understand corrosion using a *surface science* approach will be discussed. The primary focus will be internal oilfield corrosion, where dissolved CO₂/H₂S are the primary corrosive agents. More specifically, STM/LEED/XPS, supported by *ab initio* modelling, of the interaction of H₂O/CO₂/O₂/H₂S with Fe(110) will be described. STM images demonstrate that even under extremely low exposures (from an engineering perspective), significant modification of the substrate surface structure does occur, and is dependent on adsorbate identity. Intriguingly, however, for H₂O/CO₂/O₂ adsorption, XPS data indicate that the surface chemistry is apparently essentially invariant, i.e. all surfaces are simply decorated with chemisorbed O's. Data for H₂S also suggest that in the low exposure regime simple chemisorption of S occurs. In sharp contrast, much higher exposures of H₂S result in a range of surface phases, including the formation of hexagonal nano-pillars, demonstrating the complexity of the adsorption process.

Poster 1

Correlation of the optical and nanomechanical properties of C₆₀-2DM heterostructures fabricated by a hybrid electro-spray and Langmuir-Blodgett technique

Angelo Lamantia¹, Alexander J. Robson^{1,2}, Gergo Pinter¹, Kaycee L. Underwood¹, Jonathan Roberts¹, Yameng Cao¹, Ramon Bernardo Gavito¹, Robert J. Young^{1,2}, Benjamin J. Robinson^{1,2}

¹*Physics Department, Lancaster University, Lancaster, LA1 4YB, UK*

²*Materials Science Institute, Lancaster University, Lancaster LA1 4YW, UK*

(Presenting Author: a.lamantia@lancaster.ac.uk)

C₆₀ is a fascinating material due to its unusual and sometimes spectacular mechanical and optoelectronic properties, allowing a series of interesting applications in the fields of nanoscience, material science, optics and electronics [1,2,3,4]. However, since its discovery a large number of experiments have been carried out to study the intriguing properties of this exciting material but methods for preparing macroscopic quantities of monolayer C₆₀ in a facile and scalable way has proved challenging [5,6]. In addition, the combination of C₆₀ with 2D materials (2DM) are recently employed in material science in order to create new "sandwiched" structures made by alternating 2D materials (e.g. Graphene, MoS₂) with organic ultra-thin film layers. The obtained structures are particularly interesting due to the combination of the superior electronic and optical properties of 2DM with the low thermal conductivity and electrical properties of organic/molecular thin film [7–9].

Here we report a potential method for achieving monolayer (ML) production of C₆₀. We have characterised large area films produced by assembly at the air-water interface and transferred by a modified Langmuir-Blodgett (LB) method to cleaned SiO₂ substrates using a variety of scanning probe methods. We have mapped the thermal, electrical and mechanical properties with nanoscale resolution.

We investigated optimisation of the deposition through monitoring of the mean molecular area (Π - MMA) as a function of surface pressure (isotherms), Brewster angle microscopy, Raman spectroscopy and optical microscopy. Results were obtained using deionised water on a commercial KVS-NIMA trough; optimal solvent for monolayer formation was found to be toluene and methanol in 5:1 ratio by volume. C₆₀ solution was spread on the water surface using a custom built electro-spray system, enabling the formation of stable C₆₀ thin films. The transferred samples, on SiO₂ substrates, were allowed to dry in controlled atmosphere and the amount of C₆₀ on the substrate was monitored using a quartz crystal microbalance. Optical microscopy images of transferred samples showed large area coverage of the C₆₀, additionally Raman spectroscopy confirmed the presence of C₆₀ on the sample surface. The height of the obtained monolayer and its mechanical and thermal properties were measured by ultrasound force microscopy (UFM), quantitative nano-mechanics atomic force microscopy (AFM-QNM) and scanning thermal microscopy (SThM). Low noise measurements were made by TappingMode™ AFM in the new state-of-the-art ISOLAB facilities at Lancaster University. Investigations revealed a step height of about 0.76 nm ± 0.06 nm, which is in agreement with the expected molecular dimension of a single C₆₀ layer. Furthermore, measurements conducted

at the ISOLAB have shown a uniform and almost flat C₆₀ ML, suggesting that the technique is indeed a viable method for the deposition of large area ML of C₆₀ and other fullerene moieties on a hydrophilic substrate.

QNM and UFM were used to study the mechanical properties of C₆₀ ML and show a high degree of layer stability under repeated scanning, resistance to mechanical deformation and a stiffness lower than that of the SiO₂ substrate. In particular, a Young's Modulus of 7GPa was found for the obtained C₆₀ ML. Preliminary high resolution AFM measurements made in the ISOLAB have allowed us to observe the close packed molecular structure of the C₆₀ ML, and confirm that this methodology is ideally suited to the deposition of such films. The heterostructure C₆₀-2DM was realised in different step involving the mechanical exfoliation of MoS₂ from a bulk sample and a dry deterministic transfer of the obtained flake onto C₆₀ ML.

PL measurements were performed along the entire lateral size of MoS₂ flake on the top of the C₆₀ layer using a Raman spectrometer. The PL measurement enabled to access to important physical process that occur due to the interaction between C₆₀ and MoS₂. Indeed, enhancement of PL emission of MoS₂ was observed in presence of C₆₀ molecules underneath of the flake. and, this phenomena can be attributed to the p-doping effect of C₆₀ on MoS₂.

In conclusion, we present a straight forward, rapid and scalable way to produce large area ML of C₆₀ using the Langmuir-Blodgett technique as an alternative to other methods such as evaporation or drop cast film. Analysing the samples with a range of scanning probe microscopy techniques have afforded a wealth of vital information about the condition, topography and properties of C₆₀ monolayers. Combination of C₆₀ with MoS₂ has shown an interesting enhancement in the PL trion emission of MoS₂ ML in presence of C₆₀ underneath, revealing a doping effect due to the presence of C₆₀.

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Poster 2

Smart Switchable Biological Surfaces for On-demand Biosensing

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Advances in biology research and clinical diagnosis require new biological inspired tools and technology platforms to measure, understand and control biological systems. Surface confined self-assembled monolayers (SAMs) of electro-switchable peptides have the capacity to regulate biomolecular interactions in response to an applied electrical potential [1-3]. This study aims to understand the organization of charged peptides on a gold surface in order to devise switchable surfaces with the capability to control the activity of different biomolecules on-demand.

Contact angle and ellipsometry techniques were used to study the organization of SAMs comprising charged peptides, namely, oligolysines, Cys-Lys(ϵ -Lys)₄ (C5K) or Cys-Lys(ϵ -Lys)₇ (C8K) on gold, individually or in the presence of the support molecule triethylene glycol mono-11-mercaptoundecyl ether (TEG11) with different ratios.

Results on SAMs of C5K and C8K reported lower thickness values (2.37 ± 0.36 and 2.55 ± 0.77 nm) when compared with the theoretical values (4.3 and 6.8 nm). These findings suggest a flexible behavior of the peptides' backbone. In order to obtain an optimized layer, SAMs of C5K:TEG11 and C8K:TEG11 with ratios of 1:10, 1:40 and 1:100 and lastly C8K:TEG11 1:1 and 40:1 were performed. Results point to a competition between TEG11 and C5K or C8K during self-assembly. The ratios 1:10, 1:40 and 1:100 for both mixtures do not show a substantial difference or improvement in thickness. However, C8K:TEG11 40:1 reached a thickness of 3.07 ± 0.25 , showing that inverted ratios are promising. Further optimization is ongoing, with electrically-driven self-assembly.

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Poster 3

Spin and Angle-Resolved PES of Si(110)“16x2” Surfaces

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The Si(110)“16x2” surface can exist in two non-superimposable, mirror- image domains. Each of which can be prepared in enantiomerically pure form over macroscopic dimensions. These surfaces have been characterised by a number of techniques including LEED, STM and angle-resolved photoemission photoemission. We have confirmed previous LEED and STM findings and proposed a mechanism for the formation of the reconstructed surface. Further, we have undertaken spin-resolved photoemission measurements, the first results of which are indicative of a polarisation but confirmation of this requires further experimental work. Theoretical work, revealing the underlying physics behind the effect is nearing completion.

Poster 4

Supramolecular Surfaces for Protein Immobilisation

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Protein immobilisation represents nowadays one of the most challenging fields in science and many technologies have been developed basing on this idea. Biosensors, using the interaction of the protein with glucose, DNA or antibody are only a few examples of the huge amount of applications related to the concept of protein immobilisation¹. In spite of many signs of progress in the field, the best method to immobilise proteins on surfaces is still not well defined. The surface immobilisation of proteins is nowadays obtained mostly through chemical or physical adsorption. Both methods, even considering the huge amount of applications that is possible to find nowadays, still present some disadvantages. The supramolecular chemistry has the potential to overcome all these problems in a very elegant, fast and simple way by employing the host-guest interaction between a scaffold molecule and a protein². In this work, the host-guest interaction is carried out by self-assembled monolayers comprising cyclodextrin and cucurbituril moieties, which act as host molecules. On the other side, cytochrome C, insuline, α -chymotrypsin and RNase are used as representative guest proteins. So far, the presence of the host-guest complex was proved in bulk by mass spectra, in addition to a theoretical study of the complex that allows to predict the protein binding sites that will interact with our host molecules. A deeper understanding of the host-guest binding properties at surface level is required and it will be carried out by surface plasmon resonance.

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Poster 5

Surface Enhanced Raman spectroscopy of a molecular sensor for hydrogen bonding and metallization

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4-mercaptopyridine (pyS) is frequently used as sensor of protons and metal ions and as part of metal-molecule junctions in molecular electronics. Self-assembly on noble metal surfaces via the thiol group exposes the nitrogen lone pair to the solution and makes it available for coordination to metal ions or protons. This causes characteristic changes in the strong Raman response of the highly polarisable pyridine ring, particularly in the ring breathing and ring-stretching regions. Despite the widespread use of 4-mercaptopyridine as a surface enhanced Raman reporter, the spectral changes which occur on coordination of an entity to the nitrogen lone pair are still not fully understood and thus hinder the development of better sensors based on the pyridine moiety.

Here we address this issue by combining DFT calculations with experimental SERS of 4-mercaptopyridine adsorbed on a variety of gold substrates (roughened gold, nanoparticles and silica-coated nanoparticles (SHINs)), acquired with the help of a portable Raman spectrometer. We show that 4-mercaptopyridine is not just a sensor of protons, but also of species which can form hydrogen bonds to the nitrogen lone pair. In addition, using pinhole SHINs we identify a clear spectral signature of metal ion bonding. Both cases show a characteristic upshift of the ring breathing mode, due to changes in the stability of the aromatic ring upon bonding.

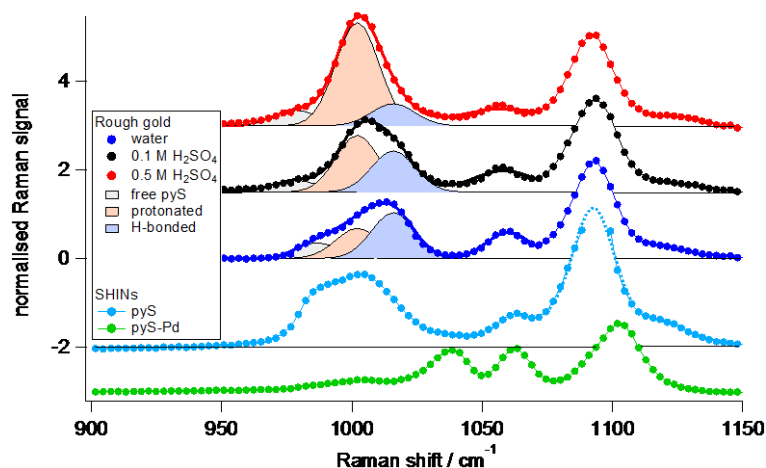


Figure 1. Influence of hydrogen bonding and metal ion coordination on the frequency of the ring breathing mode of pyS adsorbed on rough gold and silica-coated Au nanoparticles with pinholes. Pd ion coordination to the latter leads to a new ring breathing mode at 1040 cm⁻¹.

Poster 6

Self-Assembly and On-Surface Reactions of Binol Molecules on Copper Surfaces

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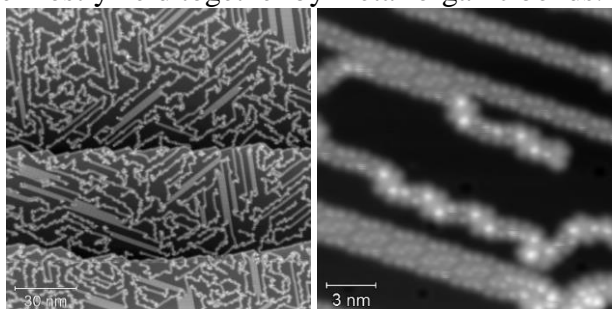
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The formation of metal-organic and covalent bonds during on-surface chemical reactions can be utilised to form strong, stable nanostructures with potential applications in nano-engineering science and technology. Many different types of structures can be formed, such as porous layers¹, linear polymers and nanoribbons². Various chemical functional groups have been utilised in efforts to create new nanostructures³.

In this study, scanning tunnelling microscopy (STM) has been used to examine the deposition of binol (1,1'-Bi-2-naphthol) molecules on a Cu(111) surface. Binol has been shown to undergo a ring closing reaction between its hydroxyl and C-H groups in solution with a copper(I) catalyst⁴, and it is believed that this may also be possible on a model surface under ultra-high vacuum.

When deposited at less than a monolayer coverage on a room temperature Cu(111) surface, the binol molecules were found to form regular clusters. Different phases of molecular self-assembly were found to occur at close to full monolayer coverage, potentially relating to the required density of packing. Upon annealing the molecules to 470K, they were observed to form nanostructures that consisted of chains and clusters, albeit of varying order. The distances between the sub-units may be consistent with either metal-organic or covalent bonding, and iron was deposited over this assembly at room temperature in order to elucidate the type of structure that had initially formed. This led to the destruction of the previously-formed chains, suggesting that they were mostly held together by metal-organic bonds.



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Poster 7

High intensity electrospray source for UHV deposition of large functional molecules for in-situ STM studies

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Electrospray ionisation beam deposition (ESI-BD) is quickly becoming a versatile technique for depositing large thermally labile molecules for study on surfaces in vacuum. The technique has been used to soft-land and analyse a wide range of molecules from fragile molecular magnets [1], to biomolecules [2] and porphyrin nanorings [3]. In this work we present a new ESI-BD instrument designed for high efficiency and high transmission, coupled with a variable temperature Scanning Tunnelling Microscope that offers the ability to study complex systems with the ultimate spatial resolution. Molecules are delivered from solution in atmospheric conditions to a sample surface located in ultra-high vacuum (UHV) by electrospray ionisation, followed by several ion optic elements that guide and mass-select ions through successive differential pumping chambers with high transmission. Additionally, the instrument is capable of generating fragment ions by collision induced dissociation (CID), which can be used to provide sequencing information of proteins and polymers. By adjusting the deposition voltage it is also possible to vary the molecule impact energy ranging from soft landing to the reactive impact regime. STM images and analysis of a selection of large molecules will be presented, demonstrating the capabilities of this scientific instrument for surface science studies.

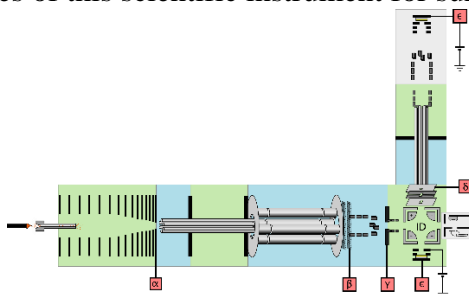


Figure 1: Schematic of the Electro Spray Ion Beam Deposition System

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Poster 8

Imaging subsurface defects in WS₂/WSe₂ CVD flakes via Ultrasonic Force Microscopies

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The implementation of two-dimensional (2D) materials has potential to revolutionise optoelectronics, energy storage, gas- and bio-sensors, photocatalysis and solar energy conversion. In particular, the atomically layered transition metal dichalcogenides (TMDCs), such as WS₂ and WSe₂ show unique electronic and optical properties, ease of manufacturing, mechanical robustness, low toxicity, as well as being composed of relatively abundant elements on Earth [1]. The growth of these materials, individually or via co-deposition by the Chemical Vapour Deposition (CVD) on the Si or SiO_x surfaces, can create complex trigonal and hexagonal structures formed by the individual layers of material, typically stacked around a single screw dislocation which defines the crystallite growth process [2].

For this research, we have used the combination of Atomic Force Microscopy (AFM) with the ultrasonic vibration – namely, the Ultrasonic Force (UFM) and the Heterodyne Force (HFM) Microscopies, for the mapping of nanomechanical properties and subsequent identification of dislocations and faults in multiple stacked WSe₂ and WS₂ layers. In UFM/HFM, the 2-8 MHz high frequency ultrasonic vibration of 1-2nm amplitude is applied to the sample, resulting in a displacement of few nm normal to its surface, causing AFM tip indentation. The hidden subsurface features such as dislocations and stacking faults have a compressibility that differs from one of the perfect sample that, in turn, modifies the dynamic mechanical impedance sensed by the AFM tip. This is detected as cantilever deflection at the kHz modulation frequency, thanks to the nonlinearity of the tip-surface interaction reflecting the hidden structure of the 2D material [3]. If both tip and sample are vibrated at the adjacent frequencies, the amplitude of the response at the difference frequency maps the subsurface nanomechanical elastic moduli, whereas the phase reflects the local dynamic relaxation processes in nanometre volumes with a time-sensitivity of few nanoseconds.

The UFM and HFM study of WS₂ and WSe₂ materials revealed a clear contrast in areas, not always linked to the topographical features, and likely reflected subsurface dislocations and stacking faults. Alternative reasons for the nanomechanical contrast - the misorientation of crystallographic axis of the layers and crystal-surface interaction are discussed. We complemented our SPM study with Raman spectroscopy to identify the distribution of the different materials in the co-grown WSe₂ and WS₂ samples. The results show that the bottom layer and the edges of the upper layer are predominantly of WS₂ and the central layers correspond to the WSe₂.

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Poster 9

Characterising inhibited interfaces using Vibrational Sum-Frequency Spectroscopy

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Corrosion mitigation in acidic conditions is most frequently achieved through the addition of organic species (corrosion inhibitors), which protect the metallic substrate by the formation of dynamic adsorbate layers. Understanding of this process, however, is rather limited, with nanoscale mechanistic detail being largely absent, and thus inhibitor selection is currently largely empirical process. Given this scenario, we are employing a novel technique, vibrational sum-frequency spectroscopy (or VSFS), in order to gain insight into such inhibited interfaces. VSFS is based on the nonlinear optical phenomenon of sum-frequency generation (SFG), wherein two photons strike a sample surface at the same spot at the same time, generating a third photon. In VSFS, these two photons (one infrared, one visible), induce a coherent combination of infrared absorption and Raman scattering, and thus the primary output from this technique is analogous to infrared absorption spectroscopy; it enables the identification of species through their vibrational signature and provides some details regarding its adsorption geometry. Crucially, however, the phenomenon of SFG can only take place when a medium possesses an inherent dipole moment, i.e., an interface between two media. This results in VSFS being interface-specific, and so spectra are not swamped by signal from bulk phases (solid, liquid or gas). Most importantly, this specificity allows VSFS to be applied in situ, and so data

can be acquired from inhibited substrates that are still immersed in a corrosive solution. Our approach to applying VSFS to substrates inhibited by nitrogen containing organic species (e.g. dodecyltrimethylammonium chloride) will be discussed, in conjunction with more conventional, quantitative techniques such as x-ray photoelectron spectroscopy.

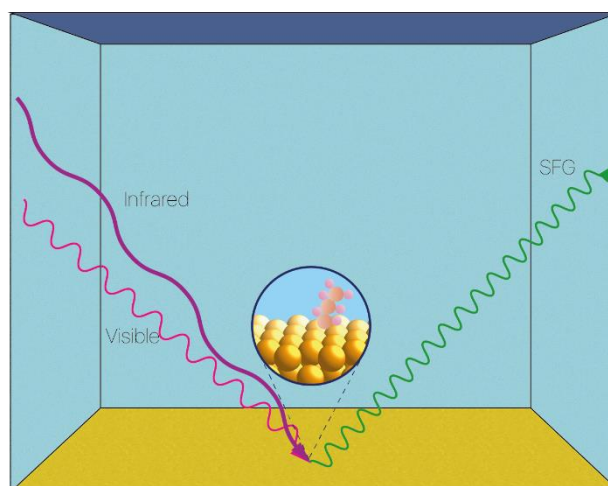


Figure 1: Cartoon illustrating phenomenon of Sum Frequency Generation

can be acquired from inhibited substrates that are still immersed in a corrosive solution. Our approach to applying VSFS to substrates inhibited by nitrogen containing organic species (e.g. dodecyltrimethylammonium chloride) will be discussed, in conjunction with more conventional, quantitative techniques such as x-ray photoelectron spectroscopy.

Poster 10

Nile red self-assembly on Au(111) surface

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Self-assembled molecular architectures on noble metal surfaces are appealing systems due to the possibility to synthesize advanced nanostructured materials and devices through molecular manipulation. The resulting features of these functional materials strictly depend on the properties of the molecules-metal interface, which in turn are tightly connected to the interaction between the particular organic-inorganic components used. Molecule-surface interactions can in fact affect the shape of the adsorbed molecules¹ and their electronic structure²⁻⁴ as well as their magnetic properties.⁵⁻⁶

Among all organic compounds, Nile Red molecules can be taken as a highly interesting model for two important reasons: i) the large flat aromatic core allowing better interactions with the substrate; ii) Nile Red is a solvatochromic dye with a strong internal dipole moment allowing to probe the effect of induced polarization on the substrate. The latter feature is involved into the control of the supramolecular architecture of the resulting monolayer film.

Taking into account all these considerations, our work investigates the Nile Red self-assembly on Au(111) surface, from sub- to mono- layer coverage. To the best of our knowledge, it is the first time that this molecular superstructure is experimentally observed on Au(111) surface. STM analysis allows to gain essential information on the molecular packing formed by molecules on the gold surface, as a function of the thermal treatments of the samples. Furthermore, the resulting interaction between the molecular assembly and the gold substrate is relatively weak as confirmed by STM investigation, while the intermolecular bond is characterized by the formation of hydrogen bond networks. This study represents a preliminary analysis that pave the way to investigation of further polar compounds on metal surfaces that are weakly interacting with the substrate. In order to gain more quantitative information about the molecules-substrates interaction and the geometry of adsorption, further investigation involving Ultraviolet and X-Ray photoelectron spectroscopy (UPS and XPS, respectively), Inverse photoemission spectroscopy (IPS) and Near edge X-ray absorption fine structure (NEXAFS) are currently in progress.

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Poster 11

Epitaxial Growth of Monolayer MoS₂ on SrTiO₃ Single Crystal Substrates

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The properties of the two-dimensional (2D) material molybdenum disulphide (MoS₂) can be manipulated by substrate engineering via the interfacial bonding. This work contributes to a fuller picture of the effects of substrate crystallinity and symmetry on the epitaxial growth of MoS₂. 2D crystals of MoS₂ are grown on the single crystal substrate strontium titanate (SrTiO₃) by chemical vapour deposition (CVD). The crystallinity of SrTiO₃ encourages crystals to grow epitaxially. The well-studied surface terminations, (111), (110), and (001) of SrTiO₃ possess completely different symmetries and lead to distinct epitaxial behaviour of MoS₂. The as-grown MoS₂ crystals are characterised by scanning electron microscopy (SEM), scanning tunnelling microscopy (STM), Raman and photoluminescence (PL) spectroscopy. On each surface of SrTiO₃, monolayer MoS₂ crystals try to develop an intimate, crystallographically well-defined contact with the substrate to maximise the interfacial bonding. To achieve this they sometimes have to distort the crystal shape and therefore partially sacrifice the lattice energy. The equilibrium shapes or orientations are also perturbed by kinetic effects such as preferential diffusion directions. The different interfacial interactions also impact the strain levels in MoS₂. Therefore, a key finding of this work is the strong interactions between MoS₂ and SrTiO₃ substrates. This steers the supported crystal shapes and orientations as determined by the epitaxial relations.

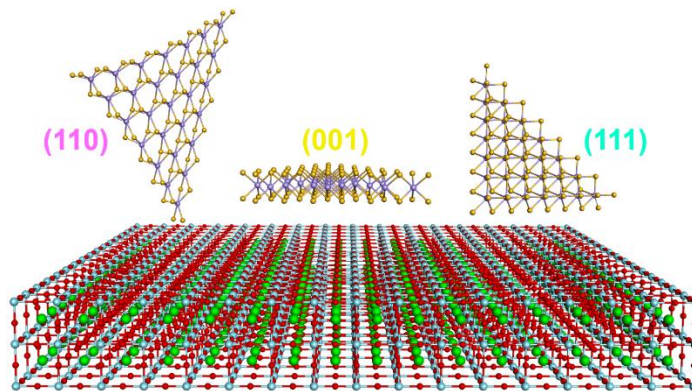


Figure 1: Atomic models of MoS₂ crystals on different surface terminations of SrTiO₃, and the model of SrTiO₃.

Poster 12

Two-Dimensional Electron Gases on the CdO Surface

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Transparent conducting oxides are of great interest for photovoltaic and optoelectronic applications as they conduct electricity whilst being optically transparent. Recently, the observation of a two-dimensional electron gas (2DEG) on the surface of several metal oxides has been reported, including CdO [1]. Previous angle-resolved photoemission (ARPES) studies of 2DEGs on the CdO have been limited by the low energy range of synchrotron beamlines, and core levels could not be measured. Here we investigate the nature of donors by studying both ARPES with low photon energies, and core levels with higher photon energies.

We studied both the naturally occurring 2DEG found on the CdO surface, and one induced by exposure to atomic hydrogen. We find the intensity of the natural 2DEG decreases with time when exposed to synchrotron radiation, during which surface species are removed from the surface. We show that the amount of species on the surface is correlated with decrease in intensity of the 2DEG, indicating that surface doping into the electron accumulation layer can be controlled by adventitious surface adsorption. We compare this 'adventitious' 2DEG with that induced by interstitial hydrogen donors [2], which we implanted by hydrogen cracking the surface.

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[2] P. D. C. King *et al.*, *Physical Review B - Condensed Matter and Materials Physics*, **79**, 035203 (2009).

Poster 13

Fibonacci modulation of a C₆₀ thin film

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The Fibonacci sequence is a mathematical series of short (S) and long (L) segments produced by a certain substitution rule, which shows no periodicity yet exhibits perfect order. This sequence can be expanded into two dimensions, producing a so-called Fibonacci square grid. Here, we demonstrate that such a mathematical grid can be reproduced in a thin film of fullerene molecules C₆₀. The 2-fold Al-Pd-Mn quasicrystal has been used as a template substrate, as its atomic surface structure is analogous to the Fibonacci grid. Mn atoms are distributed quasiperiodically across this 2D network. Adsorbed C₆₀ molecules are found in a Fibonacci grid separated by S and L lengths, corresponding to the distribution of the Mn atoms. The ratio of these lengths is consistent with the numerical value of the golden mean, τ . Both the electronic and geometric environment of the Mn atoms at the surface play a role in forming the Fibonacci grid of C₆₀. Growth of C₆₀ on a periodic phase of the same material forms a quasi-hexagonal close packed film.

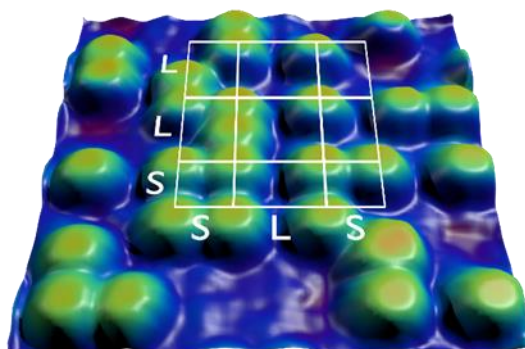


Fig. 1 – STM image of C₆₀ forming a square Fibonacci grid

Poster 14

Molecules within molecules: a NIXSW study of H₂O@C₆₀

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The encapsulation of molecules within a C₆₀ cage provides a unique environment to study their properties unperturbed by strong intermolecular interactions. Through the process of so-called molecular surgery [1, 2], a limited number of large molecules can now be encapsulated within a C₆₀ cage. In the case of fullerene-encapsulated H₂O, it has been possible to identify spin isomerisation [3] and modifications in the dielectric properties due to *ortho-para* conversion of the H₂O [4]. Despite these recent observations the precise location of the H₂O molecule within the fullerene cage, and moreover, the effect it has on the electronic properties of the fullerene molecular orbitals, remains largely unknown.

Here we describe a combined high-resolution scanning probe microscopy (SPM) and normal incidence x-ray standing wave (NIXSW) study (performed at the Diamond light source) of H₂O@C₆₀ deposited onto single crystal Cu(111) and Ag(111) samples. We show that through the use of NIXSW measurements taken using different crystal planes of the supporting Ag(111) crystal, a triangulation can be made to determine the exact position of the H₂O within the C₆₀ cage. Interestingly, we find that scanning tunnelling microscopy (STM) and non-contact atomic force microscopy (NC-AFM) show very little difference between filled and empty cages, suggesting that electronic coupling between the two molecules is minimal.

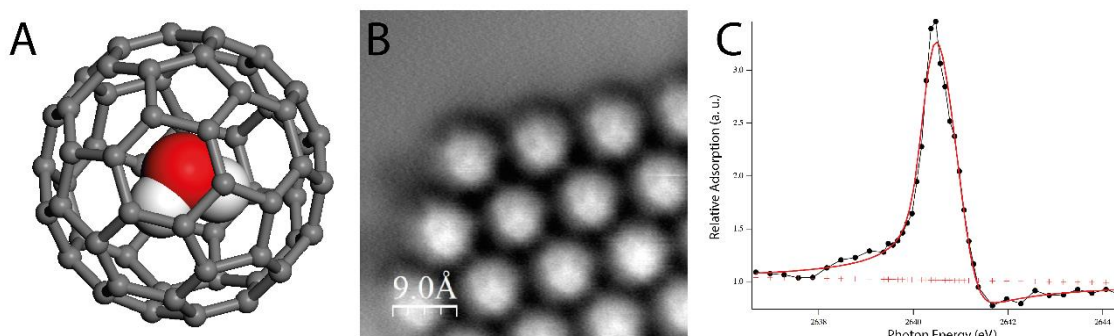


Figure 1: (A) A single water molecule encapsulated within a C₆₀ fullerene cage. (B) NC-AFM constant height frequency shift image of a mixture (as synthesized) of filled and empty C₆₀ molecules, showing an identical appearance between the two. (C) A NIXSW measurement of the O1s peak taken using the (-111) reflection of Ag(111).

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Poster 15

Nucleation, Growth and Aggregation of NbO_x Clusters on Au(111) Surfaces

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Surface-supported oxide nanomaterials are prepared by a thermally and chemically driven coalescence process. The origin of the coalescence is traced to a two-stage process. The first involves nucleation and aggregation of atomic NbO_x clusters. In the subsequent stage, the clusters are thermally driven to diffuse and coalesce to form 2D oxides. Different 2D oxide structures are organized by adjusting the oxygen potential.

Poster 16

Preparation of benzoboroxole-modified gold surfaces for selective glycoprotein recognition

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Glycans carry information in biological systems that make them an important source of biomarkers for wide range of diseases. The recognition of glycans by other molecules with high affinity and exquisite specificity, employing for instance benzoboroxoles [1], is at the heart of current and further developments in glycan-related basic research and clinically relevant diagnostics and therapeutic applications.

The aim of the research project is to create a highly sensitive and selective detection tool for glycoproteins with the use of molecular imprinting on surfaces [2]. Molecular imprinting allows the production of materials possessing specific cavities designed to provide complementing binding sites for target molecules [3].

We report optimised conditions for the most homogenous and well-packed benzoboroxole-functionalised self-assembled monolayer (SAM) on gold surfaces, which is characterized using techniques such as ellipsometry, contact angle and X-ray photoelectron spectroscopy (XPS). Preliminary studies of carbohydrate binding on the modified surfaces are performed using surface plasmon resonance (SPR).

Further work involves the molecular imprinting of benzoboroxole-glycan complexes via cross-linking on the SAM and the determination of the binding affinity and selectivity for different glycans.

Keywords: Glycans, benzoboroxoles, self-assembled monolayers.

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Poster 17

An investigation of double molecular layers of C₆₀/C₇₀ and C₇₀/C₇₀

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As the simplest fullerene molecules, research related to structural and electronic properties of C₆₀ and C₇₀ investigated. [1] They are two typical model molecules for the investigation of molecular self-assembly on surfaces. Both molecules, when deposited onto a solid substrate, have the tendency to form close-packed molecular layers. Because of the similarity between C₆₀ and C₇₀, there is an interest in exploring the possibility of making a molecular “alloy”. The different geometric shapes of the two molecules, however, seem to prevent a regular structured molecular alloy to form. [2] In addition to the idea of a molecular alloy, it is also interesting to see if a fullerene crystal can be formed with alternating layers of C₆₀ and C₇₀.

We have conducted experiments to study how a layer of C₆₀ interacts with a layer of C₇₀. The first layer C₇₀/C₆₀ is deposited on Au(111) substrate at room temperature in ultra-high vacuum. Then a partial second layer of C₆₀/C₇₀ was added. We image the molecular layers using an Omicron VT-STM. Images are acquired after the sample has been annealed to successively higher temperatures, allowing the identification of any exchange of molecules between the layers.

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Poster 18

Reversible CO₂ absorption with a superbasic ionic liquid: A near-ambient pressure X-ray photoelectron spectroscopy study

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Ionic liquids have been widely investigated as potential CO₂ capture agents. The regeneration of some ionic liquids after CO₂ capture is a relatively low energy process compared to current industrial solutions such as monoethanolamine [1, 2]. Superbasic ionic liquids, or SBILs, have received considerable attention for CO₂ capture applications due to their excellent CO₂ capacity [1]. SBILs have a deprotonated aromatic amine as the anion and their reaction with CO₂ leads to the formation of carbamate at one or more of the amine sites [3]. An additional benefit of SBILs is, unlike some other ionic liquids, do not undergo a large increase in viscosity upon CO₂ saturation, which makes them potentially useful in large-scale applications. In an experimental and theoretical study of SBILs, tetra-alkylphosphonium benzimidazolium (or [P₆₆₆₁₄][benzim]), was able to absorb equimolar quantities of CO₂ in the dry state, but when wet its capacity for CO₂ decreased [1,3]. Here we examine the absorption and reaction of the SBIL [P₆₆₆₁₄][benzim] with CO₂ and a CO₂/water vapour mixture, using near-ambient pressure X-ray photoelectron spectroscopy. Results indicate a reaction takes place between the CO₂ and aromatic nitrogen atoms to form a carbamate species. Results also appear to indicate that CO₂ preferentially binds but water blocks aromatic nitrogen sites via hydrogen bonding. The CO₂ reaction also appears to be reversible simply by evacuating the near-ambient pressure cell.

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Poster 19

Strategies for molecular imprinting of prostate cancer biomarkers on Au substrates – adapting surface chemistry to clinical diagnostics

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The diagnosis of prostate cancer (PCa) relies on the outdated biomarker prostate specific antigen (PSA) which significantly lacks clinical sensitivity and specificity. It is recognised that detection of aberrant glycosylation on the PSA biomarker would substantially improve both diagnosis and provide prognosis due to relation between glycosylation changes and aggressive malignancy. We propose a novel method of molecular imprinting utilising boronic acids (BA) to provide a reusable surface for detection of specific PCa associated glycoforms of PSA. (1,2) Our assay relies on two stages: the formation of a stable self-assembled monolayer (SAM) modified with terminal alkyne or acryloyl groups through thiol-Au interactions and the complexation of BA to PSA glycans and subsequent polymerisation to the monolayer. SAM formation uses modified 3,3'-dithiodipropionic acid, 11-mercaptoundecanoic acid or L-cysteine to generate monolayers of varying thickness and packing on Au substrates. Glycan chains on cancer derived PSA (caPSA) are then complexed to 3-((azidomethyl)phenyl) boronic acid or 3-(acrylamido)phenyl boronic acid through reversible covalent BA-saccharide interactions which are then polymerised to the SAMs through click or free radical mechanisms. An inert heptaethylene glycol is then polymerised around immobilised caPSA and the PSA washed from the surface to provide a pocket specific to PSA dimensions lined with complimentary boronic acids to caPSA glycan structures (*Fig. 1*).

Modified SAM compounds have been synthesised in house and stable SAMs of L-cysteine have been produced and imprints capable of differentiation between glycoprotein standards RNase B and A. The packing and stability of alternative SAM compounds for producing clinically relevant imprints will be examined with similar techniques including ellipsometry, contact angle, X-ray photoelectron spectroscopy and surface plasmon resonance studies.

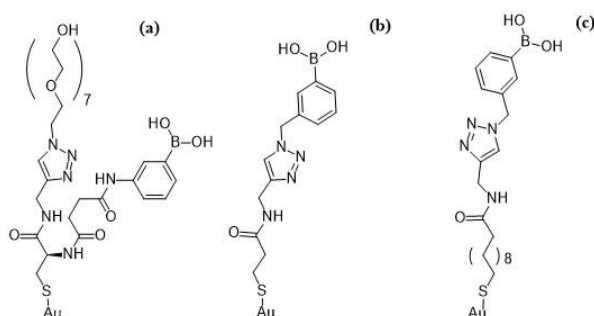


Fig. 1 Chemical structures of polymerised imprint constituents (a) acryloyl/alkyne L-cysteine (b) alkyne 3,3'-dithiodipropionic acid, (c) alkyne 11-mercaptoundecanoic acid.

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Directions/car parking

Address:

Victoria Gallery & Museum
Ashton Street
University of Liverpool
Liverpool
L69 3DR

By Road:

Postcode for satellite navigation systems: L3 5TR

From the M62: at the end of the motorway continue straight ahead on to Edge Lane (A5080 and A5047) and follow the signs for Liverpool city centre and the University.

By Rail:

The nearest mainline station is Liverpool Lime Street. The nearest local station is Liverpool Central.

Use the Merseyrail website or National Rail Enquiries to plan your journey.

By Bus:

From the City Centre buses 14 and 79 go up Brownlow Hill approximately every 5 minutes. The buses leave from the side of the Adelphi Hotel at the bottom of Brownlow Hill and stop outside the Victoria Gallery & Museum at the top of Brownlow Hill.

Car parking:

There is no on-site parking at the VG&M but there are several pay and display car parks situated close by.

- University of Liverpool Visitor car park situated on Mount Pleasant, next to the Sports Centre : Sat Nav: L35TR OR on Brownlow Street: Sat Nav: L35DA. (£2 for 1 hour, £3 for 2 hours, £6 all day to 5.30pm). Note that these will most likely be full from early morning.
- Mount Pleasant National Car Park (£1 for 1 hour, £4 all day) : Sat Nav: L3 5SD.
- Liverpool Metropolitan Cathedral Car Park (£1 for 1 hour, £2 for 2 hours, £5 all day to 6.00pm): Sat Nav: L3 5TQ.

Map

