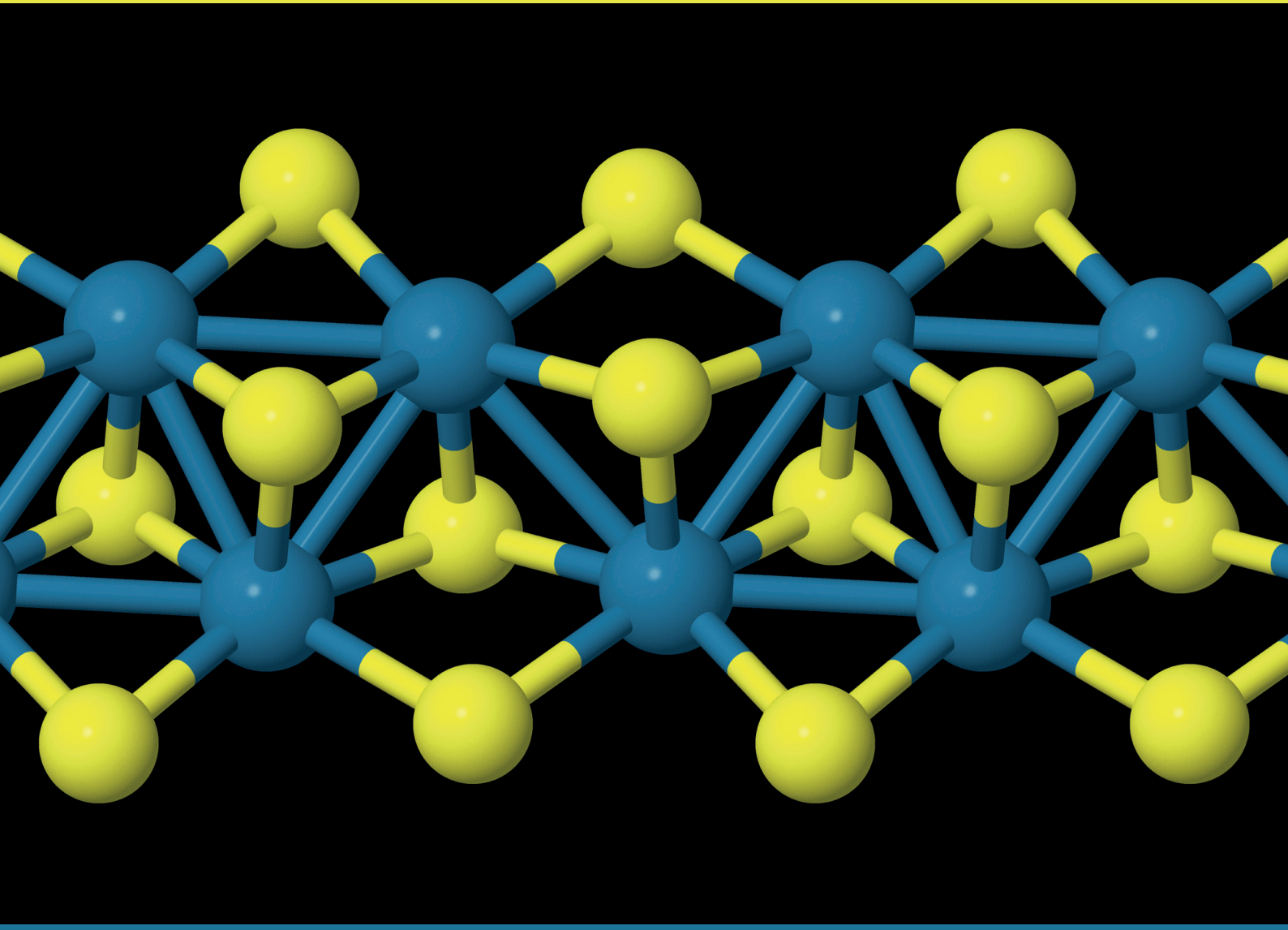
Programme and Abstracts



TMD-UK

1–2 September 2016
University of Bath, Bath, UK

IOP Institute of Physics

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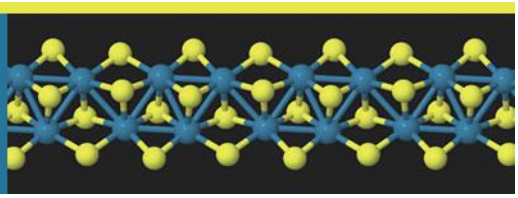
TMD-UK

1–2 September 2016, University of Bath, Bath, UK

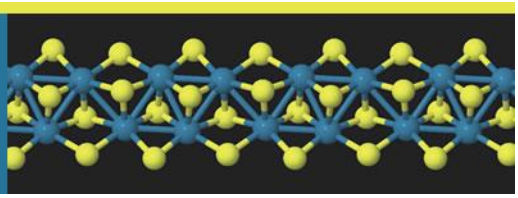


Content

IOP Institute of Physics

TMD-UK

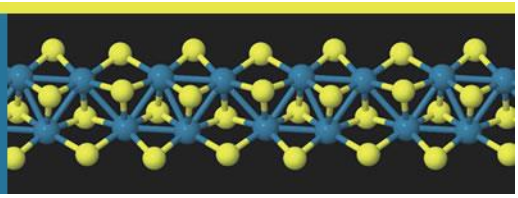
1–2 September 2016, University of Bath, Bath, UK



PROGRAMME

Thursday 1 September

11:30	**Registration**
12:00-13:00	**Lunch**
	All lectures will take place in the Chancellors' Building 2 in the University of Bath
	Session 1
13:00	**Welcome** – Dr Daniel Wolverson, University of Bath
13:15	**(Invited) Excitonic effects and spin-valley physics in monolayer transition metal dichalcogenides** Dr Bernard Urbaszek, Université de Toulouse, France
14:00	**3D Structures integrated with MoS_2** Katrina Morgan, University of Southampton, UK
14:15	**Direct light extraction from 2D materials using liquid micro-lenses** Christopher Woodhead, Lancaster University, UK
14:30	**Quantum dots in MoS_2 defined using atomic force microscope lithography** Alice Sackville Hamilton, University College London, UK
14:45	**Exploring 2D heterostructures as highly sensitive photodetectors** Jake Mehew, University of Exeter, UK
15:00	**Electrically pumped quantum emitters in van der Waals heterostructures** Luca Sortino, University of Sheffield, UK
15:15	**Refreshment break and posters - Chancellors' Building 2.6 foyer**
	Session 2
15:45	**(Invited) Structure and properties of large area 2D transition metal dichalcogenides grown by chemical vapour deposition** Professor Jamie Warner, University of Oxford, UK
16:30	**Chemical functionalisation of 2H-Phase transition metal dichalcogenides** Mark Bissett, The University of Manchester, UK
16:45	**Identifying the two vertical orientations of the rhenium dichalcogenides** Lewis Hart, University of Bath, UK
17:00	**WS_2 nanowires, 2D nanomeshes, and 2D in-plane films through one single CVD route** Zichen Liu, University of Bath, UK



17:15 **Refreshment break and posters**

17:45 **CVD growth of 2 dimensional MoS_2 and heterostructures with graphene**
Ravi Sundaram, Oxford Instruments Plasma Technology, UK

18:00 **Epitaxial templating of 2D metal chlorides on monolayer MoS_2**
Shanshan Wang, University of Oxford, UK

18:15 **A facile topochemical route to the production of strictly 2D transition metal dichalcogenide materials**
David Moran, University of Glasgow, UK

18:30 **Ultrathin 2D Opto-electronics based on CVD grown crystals**
Haijie Tan, University of Oxford, UK

18:45 **In-situ atomic level observation of edge terminations of monolayer MoS_2 at elevated temperatures**
Qu Chen, University of Oxford, UK

19:00-19:30 **Poster session and drinks reception - Chancellors' Building 2.6 foyer**

19:30 **Free time for delegates to explore the City of Bath**

Friday 2 September

08:30 **Registration - Chancellors' Building 2.6 Foyer**

Session 3

09:00 **(Invited) Photonics and polaritonics with van der Waals heterostructures**
Professor Alexander Tartakovskii, University of Sheffield, UK

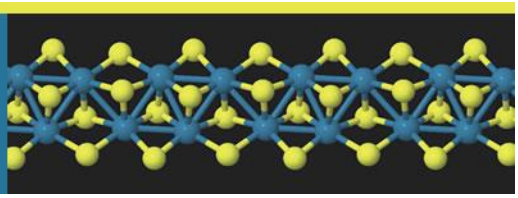
09:45 **Interlay excitons in van der Waals heterostructures**
Evgeny Alexeev, University of Sheffield, UK

10:00 **Large scale CVD 2D heterostructures**
Nikos Aspiotis, University of Southampton, UK

10:15 **Resonantly excited exciton dynamics in two-dimensional MoSe2 layers**
Lorenzo Scarpelli, Cardiff University, UK

10:30 **Deterministic localisation and resonant laser spectroscopy of quantum emitters in mono- and bi-layer WSe_2**
Art Branny, Heriot Watt University, UK

10:45 **Room temperature Tamm-Plasmon Exciton-Polaritons with a WSe_2 monolayer**
Nils Lundt, University of Wuerzburg, Germany



11:00 **Refreshments and posters - Chancellors' Building 2.6 Foyer**

Session 4

11:30 **(Invited) Direct k-space imaging of spin-valley locking in transition-metal dichalcogenide semiconductors and superconductors**
P D C King, University of St Andrews, UK

12:00 **Determination of band offsets, hybridization and exciton binding in 2D semiconductor heterostructures**
N R Wilson, University of Warwick, UK

12:15 **Linear-scaling DFT simulations of layered material heterostructures**
Nicholas Hine, University of Warwick, UK

12:30 **Band-structure effects in vertical layered-material heterostructures**
Gabriel Constantinescu, University of Cambridge, UK

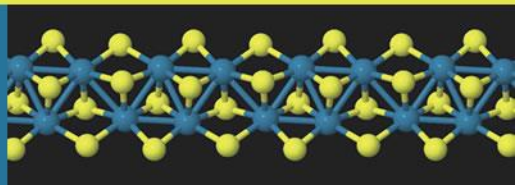
12:45 **Suppression of inter-valley relaxation in monolayer WSe_2 with small magnetic fields**
Tom Lyons, University of Sheffield, UK

13:00 **Cavity enhanced light extraction from monolayer topological defects**
Yameng Cao, Lancaster University, UK

13:15 **3D printing of MoS_2 nanosheets**
Cecilla Mattevi, Imperial College London, UK

13:30 **Closing summary**

13:45 **Packed Lunch to take away**



Poster Programme

P.1 **Optoelectronic properties study of atomically thin ReSSe with weak interlayer coupling**
Viktor Zólyomi, The University of Manchester, UK

P.2 **Uniform growth of a wafer scale MoS_2 monolayer using chemical vapor deposition (CVD)**
Omar Omar, University of York, UK

P.3 **ARPES study of intercalated bulk MoS_2 superconductors**
Mohammed Bin Subhan, University College London, UK

P.4 **Tuning correlated electron states in few-layer 2H-TaS2 by field-effect gating**
Hasti Shajari, University of Bath, UK

P.5 **Controlled formation of an isolated miniband in bilayer graphene on an almost commensurate $\sqrt{3}$ x $\sqrt{3}$ substrate**
Damien Leech, University of Bath, UK

P.6 **Linear-Scaling DFT investigations of defect formation energies within TMDC lateral heterostructures**
Nelson Yeung, University of Warwick, UK

P.7 **Growth and characterisation of $TiSe_2$: A chiral charge density wave material**
Charles Sayers, University of Bath, UK

P.8 **High photoresponsivity in graphene-multilayer WS_2 heterostructures with an ionic polymer gating**
Selim Unal, University of Exeter, UK

P.9 **Computational study of the effect of single point defects on the electrical properties of MoS_2 bilayer**
Pedro Derosa, Louisiana Tech University/Grambling State University, USA

P.10 **Low wavenumber Raman determination of layer number in ReS_2 flakes**
Tim Batten, Renishaw plc, UK

P.11 **Rhenium disulphide and rhenium diselenide: lattice dynamics in anisotropic layered semiconductors**
Daniel Wolverson, University of Bath, UK

P.12 **First-principles lattice dynamics of monolayer MoS_2**
Daniel Wolverson, University of Bath, UK

P.13 **nanoARPES of 2-dimensional TMD heterostructures**
Natalie Teutsch, University of Warwick, UK

P.14 **AACVD routes to tungsten disulfide on graphene**
Daniel Wolverson, University of Bath, UK

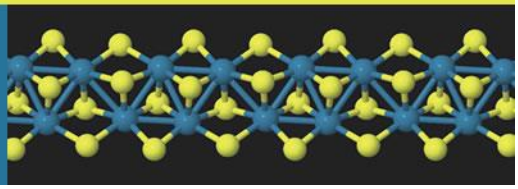
P.15 **Inorganic graphene materials: Novel precursors for TiS_2, ZrS_2 and HfS_2 production**
Daniel Wolverson, University of Bath, UK

P.16 **Defects and dopants in WSe_2 and their local electronic characterization**
Adelina Ilie, University of Bath, UK

P.17 **Topological ladder in the metallic TMD 1T-PdTe2**
O Clark, University of St Andrews, UK

P.18 **Spin-valley locking in the normal state of a transition-metal dichalocogenide superconductor**
L Bawden, University of St Andrews, UK

P.19 **Dipolar exciton-polaritons in electric and magnetic fields**
Joe Wilkes, Cardiff University, UK



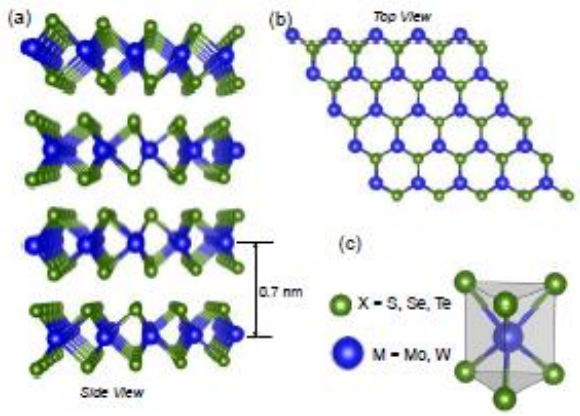
Abstracts

(Invited) Excitonic effects and spin-valley physics in monolayer transition metal dichalcogenides

B Urbaszek

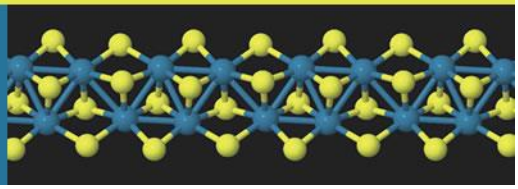
Université de Toulouse, France

Transition metal dichalcogenides such as WSe_2 and MoS_2 are layered semiconductors, with strong in-plane bonds and Van-der-Waals bonding between the individual layers. Although indirect semiconductors in bulk form, when thinned down to one monolayer they become direct semiconductors in the visible to the near infra-red region of the optical spectrum [1]. These atomically flat 2D materials have unique physical properties for manipulating electrons in non-equivalent valleys in momentum space [2] and can potentially serve as building blocks in Van-der-Waals heterostructures for optoelectronics applications [3].



In this talk we will discuss the intriguing linear and non-linear optical properties of monolayer transition metal dichalcogenides governed by robust excitons [4], Coulomb bound electron-hole pairs with binding energies of 500 meV. We investigate experimentally the competition between optically bright and dark excitons that determines the light emission yield in these binary materials and their ternary alloys $Mo_{(1-x)}W_xSe_2$ [5]. We discuss valley state manipulation with polarized lasers and the numerous open questions and challenges in this fast growing field.

[1] Mak et al, PRL 105, 136805 (2010); Lezema et al NanoLett 15, 2336 (2015)
[2] Di Xiao et al, PRL 108, 196802 (2012)
[3] Rivera et al, Science 351,688 (2016)
[4] Wang et al, PRL 114, 097403 (2015) & Lagarde
[5] Wang et al, Nat. Comms. 6, 10110 (2015)



3D Structures Integrated with MoS_2

K A Morgan[1], X Zheng[2], Y-L D Ho[2], M P C Taverne[2], L Chen[2], C-C Huang[1], N K Aspiotis[1], I Zeimpekis[1], J G Rarity[2] and D W Hewak[1]

[1]University of Southampton, UK, [2]University of Bristol, UK

Photonic crystals (PC) are fabricated using a polymer 3D structure coated with a thin molybdenum disulphide (MoS_2) layer resulting in a polymer-high refractive index composite. A two-step process is used; 3D polymer woodpile structures are fabricated by direct laser writing (DLW) followed by chemical vapour deposition (CVD) of MoS_2. The high refractive index contrast between polymer-MoS_2 and air results in a photonic band gap for centre wavelength=1.27um at normal incident.

Introduction: Periodic crystal structures interact with light, creating a full photonic band gap (PBG), stopping the propagation of a specific wavelength (similar to the periodicity) in all directions. Inserting a defect into a PC creates an optical micro-cavity with confinement exceeding 2D slabs/waveguides due to reduced scattering and out-of-plane radiation losses [1].

Inserting an emitter into the cavity creates a single photon source, if the photon wavelength emitted is equal to the PBG. With strong coupling between cavity photons and two-level systems, cavity quantum electro dynamics (cavity-QED) is achieved.

Fabrication: Previously, 3D PCs are fabricated using a 2D layer-by-layer lithographic technique, with limited number of stacks [2]. More recently 3D structures are fabricated using a two-photon polymerisation (2PP) technique using DLW.

In this work we demonstrate 3D PC structures fabricated initially from polymer using 2PP, on a Nanoscribe Photonic Professional DLW system. A body-centred-cubic woodpile structure is fabricated, consisting of layers of parallel dielectric rods, with perpendicular layers, with and without walls [1]. CVD is then used to coat the structure in MoS_2; a high refractive index transition metal di-chalcogenide (TMDC). Firstly, a chlorine-based precursor ($MoCl_5$) is reacted with H_2S at room temperature. A second annealing step converts the film into MoS_2, reducing excess sulphur and Cl [3]. Due to polymer temperature constraints, 250° C is chosen. Conformal coverage was achieved throughout the structures as seen in Figure 1, with no damage.

The MoS_2 thickness is 10.0nm, measured by surface profiling and ellipsometry, as shown in Figure 2, with n=3.0 and k=0.78 at 632.8nm. Raman spectra, shown in Figure 3, reveal the two MoS_2 characteristic vibrational modes.

Photonic Band Gap Measurements: Figure 4 shows the measured photonic band gap before and after 10nm MoS_2 coating. The reflectance is measured using S-polarized white light source. A broadening and red shift of photonic band is observed. The measured reflectance at normal incident is shown in Figure 5. The full width at half maximum (FWHM) of photonic band gap is increased by 34nm after coating with MoS2. The reflectance at a higher incident angle 11o before and after MoS_2 is illustrated in Figure 6.

[1] Taverne M et al., 2015 J.Opt.Soc.Am.B 32, 639-648
[2] Deubel M et al., 2004 Nat.Mat. 3, 444-447
[3] Huang C-C et al., 2014 Nanoscale 6, 12792-12797

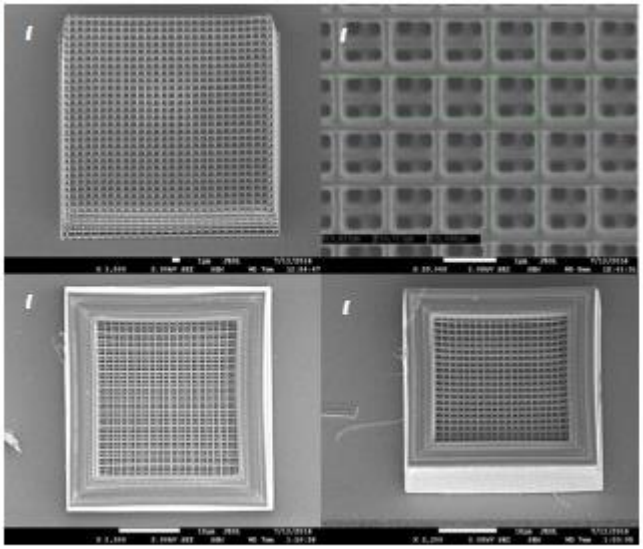


Figure 1. SEM images of BCC Woodpile Structures coated in 10nm of MoS2 with (a) no walls with tilted view, (b) higher magnification to show woodpile structure, (c) structure with walls for structural support and (d) structure with wall with tilted view.

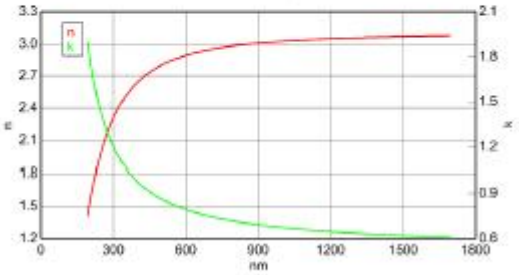


Figure 2. Refractive index and absorption vs. wavelength measured by ellipsometry for MoS_2 on 300 nm SiO2/Si.

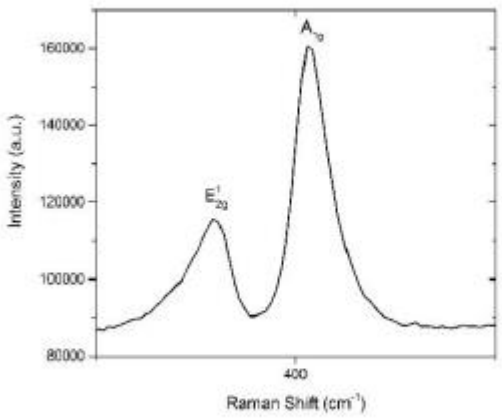


Figure 3. Raman spectra of MoS_2 vibrational modes, on quartz substrate. Peak separation is 23.4 cm^{-1}.

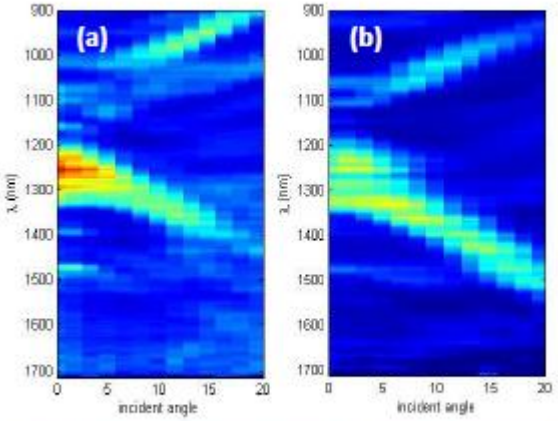


Figure 4. Measured angular reflectance of BCC woodpile structures (a) before coating (b) after coating

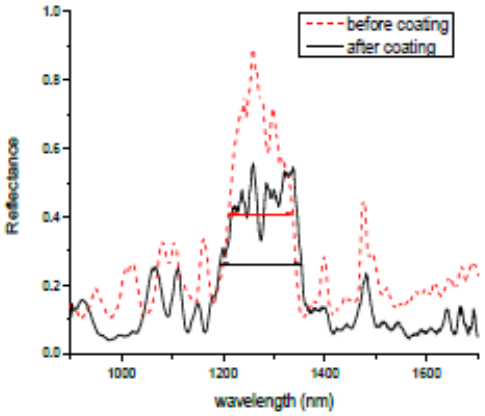


Figure 5. Measured reflectance at normal incident angle before and after coating.

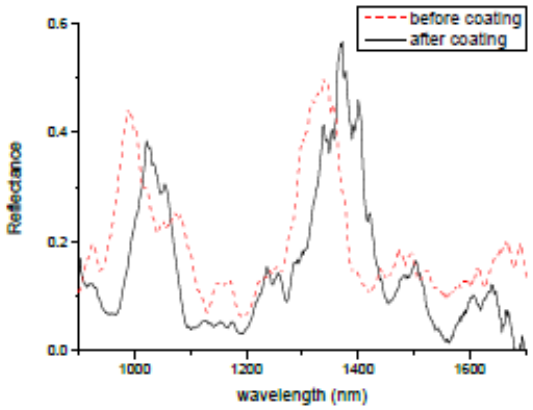


Figure 6 Measured reflectance at incident angle 11° before and after coating.

Direct light extraction from 2D materials using liquid micro-lenses

C Woodhead[1], J Roberts[1], Y Noori[1], Y Cao[1], R Bernardo-Gavito[1], P Tovee[1], A Kozikov[2], K Novoselov[2] and R J Young[1]

[1]Lancaster University, UK, [2]The University of Manchester, UK

Direct bandgap 2D semiconductor materials such as monolayers of transition metal dichalcogenides (TMDCs), show great promise in optoelectronic devices enabling exciting new technologies such as ultra-thin quantum light LED's[1]. These structures can have incredible advantages, enabling almost seamless integration into conventional silicon structures. However, extracting light out of these structures can be a challenge, often requiring costly and time consuming processing e.g. engineered waveguides or cavities[2]. Furthermore none of these methods allow you to observe the light directly, therefore a cheap and simple solution can be vital in devices where direct observation is necessary[3].

Solid immersion lenses (SILs) have previously been used to increase light out of semiconductor nanostructures[4]. We applied this idea to TMDC materials by bonding a SIL formed from a UV curable epoxy; this increases light collection and protects the SIL from damage/degradation caused by exposure to ambient conditions. Our studies revealed that a SIL can greatly enhance the photoluminescence of WSe_2 by up to 6x (more than theory predicts for a SIL of this shape), without effecting the wavelength. However we also found that the epoxy appears to reduce the emission of the MoS_2, suggesting that there could be doping effects due to the epoxy. Overall this method shows great promise as a cheap, and scalable method for enhancing the efficiency of WSe_2 based devices.

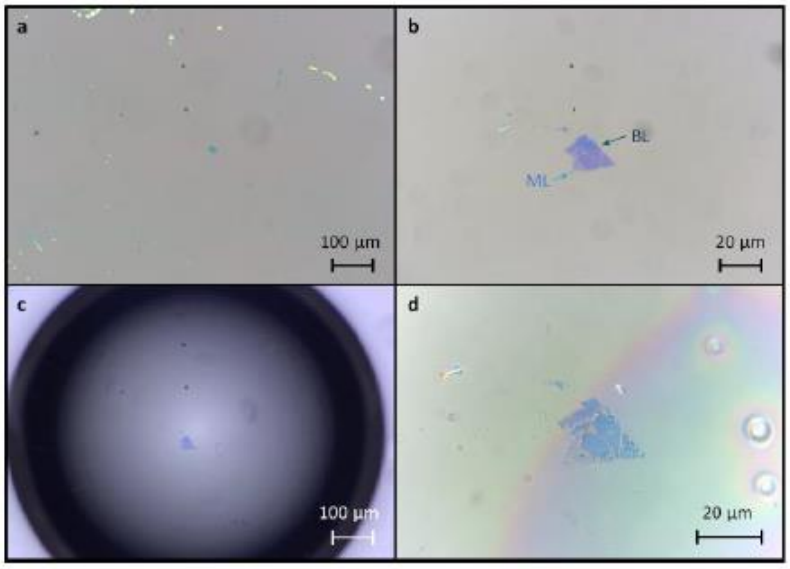


Figure 1. Optical microscope image showing an isolated monolayer of WSe_2, before (a,b) and after (c,d) mounting a SIL; the scale bar in (d) has been adjusted to account for the SIL's magnification.

[1] Berraquero, C. P. et al. Atomically thin quantum light emitting diodes. arXiv, 160308795P (2016).
[2] Xia, F, et al. A. Two-dimensional material nanophotonics. Nat Photon 8, 899-907, (2014).
[3] Roberts, J. et al. Using Quantum Confinement to Uniquely Identify Devices. Sci Rep 5, 16456, (2015).
[4] Serrels, K. A. et al. Solid immersion lens applications for nanophotonic devices. NANOP 2, 021854,(2008).

Quantum dots in MoS_2 defined using atomic force microscope lithography

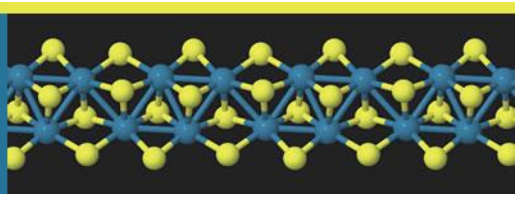
A Sackville Hamilton[1], A Iglesias del Dago[2], M O'Brien[3], G Duesberg[3], R Garcia[2] and M Buitelaar[1]

[1]University College London, UK, [2]Instituto de Ciencia de Materiales de Madrid, Spain, [3]Centre for Research on Adaptive Nanostructures and Nanodevices, Ireland

Here we present a flexible method for fabricating quantum dots in MoS_2. Atomic force microscope lithography (AFML) is used to define a dot by locally oxidising the area around the dot, creating an insulating barrier. The I-V characteristics of the device can be monitored during lithography, and the dot dimensions adjusted accordingly.

The success of the oxidation, and the quality if successful, depends on the relative humidity inside and outside the AFM chamber, and the cleanliness of the MoS_2 surface.

When MoS_2 crystals are contacted using photolithography or electron beam lithography, the surface of the device is contaminated with resist residue. As well as affecting the quality of AFM oxidation, these residues can also alter the electrical properties. Various methods of complete resist removal have been reported and tried with unsatisfactory results, including annealing [1], and scraping the surface using a contact mode AFM tip [2]. A preferable contacting solution which is resist-free is shadow mask evaporation [3]. Masks down to 4 µm separation have been fabricated.



Preliminary room temperature and low temperature transport measurements performed on the above devices are also presented.

[1] S.D. Namgung et al., Influence of post-annealing on the off current of MoS2 field-effect transistors, Nanoscale Research Letters (2015) 10:62; DOI 10.1186/s11671-015-0773-y
[2] A.M. Goossens et al., Mechnical cleaning of graphene, Applied Physics Letters (2012) **100**, 073110; DOI 10.1063/1.3685504
[3] W. Bao et al., Lithography-free fabrication of high quality substrate-supported and freestanding graphene devices, Nano Research (2010) 3: 98-102; DOI 10.1007/s12274-010-1013-5

Exploring 2D heterostructures as highly sensitive photodetectors

J D Mehew, S Unal, E Torres Alonso, M F Craciun and S Russo

University of Exeter, UK

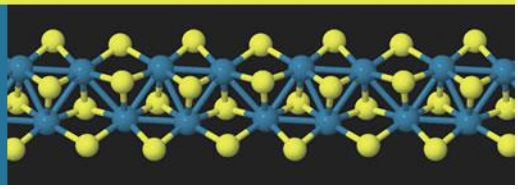
Photodetectors are essential components of modern electronics which are utilised in many communication, imaging, and sensing applications. Typically they compose of a semiconductor, such as silicon, as these exhibit strong absorption across the visible electromagnetic spectrum. Whilst these traditional photodetectors currently dominate the market, the requirements are constantly changing with demand for smaller, more lightweight and more efficient devices.

Graphene and related materials can function at the ultimate thickness limit, a monolayer, thus provide immediate advantages over their bulkier counterparts as they demonstrate remarkable mechanical strength and flexibility. These 2D materials have been shown to possess a host of different electrical and optical properties depending on the choice of material and number of layers.[1] Graphene, for instance, is optically transparent and has high charge carrier mobility, whereas, Tungsten Disulphide (WS_2), as a gapped semiconductor, has strong light absorption in the visible range.

Fabricating a van der Waals heterostructure from these materials allows their favourable properties to be combined. 2D photodetectors assembled in this manner use graphene as the charge transfer layer and a semiconductor as the optically active material resulting in highly photoresponsive devices. Currently these devices are limited by slow response times making them unsuitable for most imaging applications.[2-5]

In this work we manage to overcome these limitations through the deposition of an ionic polymer gate on top of heterostructures of WS_2 and graphene. The optoelectronic properties of our heterostructure photodetectors far surpass those of the constituent materials. We report responsivities of 10^6A/W and response times many orders of magnitude faster than other hybrid graphene photodetectors owing to this unique gating strategy. These properties make our photodetectors suitable for high frame rate video imaging applications which we have demonstrated by creating a prototype camera.

The significant improvement in device performance compared with previous graphene heterostructure photodetectors means that these results will be of interest to both those working in industry on commercial imaging applications and as well as the wider academic community. For the latter group it is also noteworthy that with these devices we have been able to observe exciton behaviour in WS_2 through photocurrent measurements without the need for low temperatures or suspended devices. This could offer researchers a new avenue in which to explore exciton physics at the nanoscale.



[1] Q.H. Wang et al., Nat. Nanotechnol. 7, 699 (2012)
[2] G. Konstantatos et al., Nat. Nanotechnol. 7, 363 (2012)
[3] S.Y. Chen et al., Carbon N. Y. 63, 23 (2013)
[4] K. Roy et al., Nat. Nanotechnol. 8, 826 (2013)
[5] W. Zhang et al., Sci. Rep. 4, 3826 (2014)

Electrically pumped quantum emitters in van der Waals heterostructures

L Sortino[1], S Schwarz[1], F Withers[2], J K Maguire[1], A P Foster[1], S Dufferwiel[1], L Hague[2], A Kozikov[2], M N Makhonin[1], L R Wilson[1], K S Novoselov[2] and A I Tartakovskii[1]

[1]University of Sheffield, UK, [2]University of Manchester, UK

Van der Waals heterostructures allows to combine the unique properties of two-dimensional materials to produce functional optoelectronic devices [1-2]. Recently, quantum emitters have been reported in atomically thin layers of transitional metal di-chalcogenide (TMDC) WSe2 [3-7]. Here we demonstrate the luminescence under electric charge-injection of a defect emitter in a light-emitting device (Fig. 1a) consisting of a vertical heterostructure of a single layer of TMDC, hexagonal boron nitride (hBN) and graphene [8]. This design allows the vertical injection of carriers from graphene contacts into the active material, with hBN acting as a tunneling barrier (Fig. 1b). The spectroscopic analysis of the electroluminescence from these localized emitters is shown Fig 1c. At low voltage, the quantum dot emission is dominant, while at higher voltage excitonic features appear.

The adaptability of van der Waals heterostructures on arbitrary substrates, and the electric control of quantum light sources, makes these devices new candidates for the integration with existing optoelectronic and photonic systems.

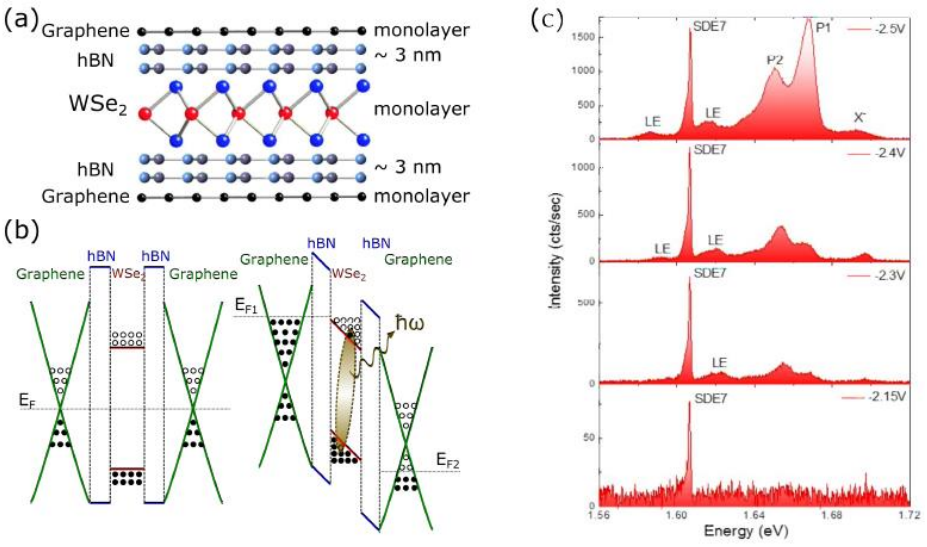


Figure 1: (a) Schematic of the electrically pumped light-emitting device. (b) Band structure of the device with and without applied bias voltage. (c) Emission spectra at different applied bias voltage.

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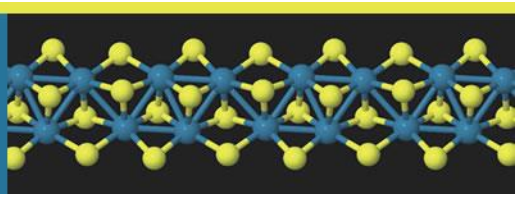

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(Invited) Structure and properties of large area 2D transition metal Dichalcogenides grown by chemical vapour deposition

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Monolayer 2D transition metal dichalcogenides offer semiconducting properties that expand the application of 2D materials beyond graphene and h-BN. A key element to their realization in technology will be the ability to grow large areas with control over layer number and grain size. I will discuss our recent work on growing both MoS2 and WS2 by CVD, as well as heterostructures of TMDs on graphene and BN using all CVD methods. The atomic structure of their defects are directly imaged using aberration-corrected transmission electron microscopy. The photoluminescent properties of monolayer TMDs are highly sensitive to local doping and interactions with other materials. I will discuss recent work on understanding the effects of substrate doping and charge transfer in vertical stacked heterostructures as well as integrating with molecular dopants.

Chemical functionalization of 2H-Phase transition metal dichalcogenides

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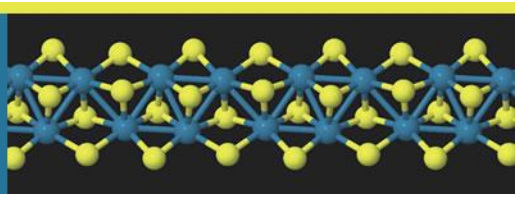
The University of Manchester, UK

Chemical functionalization of two-dimensional (2D) materials provides an ideal route to modify their mechanical and electronic properties. Previously, there has been a wide variety of studies into the functionalization of graphene, which has led to control over the electronic structure through doping, as well as modifying the mechanical properties when used in composites. One well established method for functionalizing carbon systems is through the covalent reaction of aryl diazonium moieties. However, similarly structured inorganic 2D materials such as transition metal dichalcogenides (TMDs) have generally been considered to be chemically inert, with few studies into the covalent modification and functionalization of them. By establishing a versatile and simple method of covalently modifying exfoliated TMDs it will be possible to greatly expand their suitability for a myriad of applications including composites and electronics.

Here we present a method for covalently modifying several TMDs (MoS_2, WS_2, $MoSe_2$, and WSe_2), which have been exfoliated via ultrasonication in solvent, with strong electrophilic aryl diazonium salts such as 4-nitrobenzenediazonium (4-NBD) and 4-bromobenzenediazonium (4-BBD). The use of solution phase exfoliated crystals allows for easily scalable and versatile solution based processing. The successful modification of the TMD crystals was investigated using a variety of techniques including; optical absorption, Raman and infra-red spectroscopy as well as XPS. Previously, only the metallic 1T-phase of MoS_2, produced by lithium intercalation, has been shown to be reactive with aryl diazonium molecules [1]. However, due to the high edge density from the small crystallite size (~300 nm) and basal defects which are possibly created during the ultrasonication process, we are



able to successfully covalently modify the much more common semi-conducting 2H-phase of both sulfide and selenide containing TMDs. The successful functionalization was also compared to mechanically exfoliated MoS_2 crystals to investigate the effect of layer number on the reactivity.

The chemically modified TMD crystals were then incorporated into several applications such as polymer composites, where the effect of functionalization on the interfacial strain transfer within a polymer matrix was measured. The materials were also tested in energy storage devices, where the effect of doping on the electronic structure affected conductivity and electrochemical performance was investigated.

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Identifying the two vertical orientations of the rhenium dichalcogenides

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University of Bath, UK

The rhenium dichalcogenides, rhenium disulphide (ReS_2) and rhenium diselenide ($ReSe_2$), are two of the lesser known transition metal dichalcogenides, (TMDs) explored by Yoffe et al[1]. Unlike the better known TMDs, molybdenum disulphide and tungsten disulphide, these materials are not stable in the 1T or 2H phase but are instead found in a distorted 1T phase. These materials may be of use when designing new electronic devices from van der Waals heterostructures[2]

A unique feature of these materials is that there are bonds found between the transition metals, with the rhenium atoms forming quasi-one dimensional “diamond” chains. Along the direction of these chains the conductance is largest[3]. With these materials having anisotropic properties it is important to be able to identify the orientation and we have shown here that Raman spectroscopy is an ideal tool for this[4].

The act of flipping a flake, that is a C_2 rotation about the in-plane axis, is not a symmetry that belongs to these materials. This means that we expect two inequivalent vertical orientations. We have shown that it is possible to identify which “way up” the material is using polarised Raman spectroscopy[5]. There have been a few reports on the CVD growth of these materials[6,7] and our work will be important when understanding the growth of the rhenium dichalcogenides as it is expected that domains having both of these orientations will be present, along with new type of grain boundaries between them.

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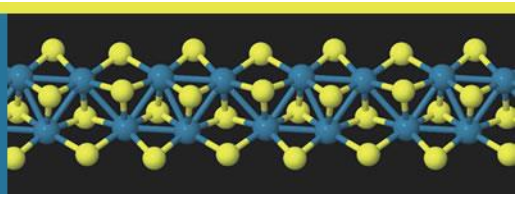

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WS_2 nanowires, 2D nanomeshes, and 2D in-plane films through one single CVD route

Z Liu and A Ilie

University of Bath, UK

A variety of bottom-up growth processes for transition metal dichalcogenide (TMDs) layers have been proposed and demonstrated in recent years. For WS_2, one such growth process uses chemical vapour deposition (CVD) in conjunction with tungsten oxide and sulphur as precursors. Here we demonstrate a CVD route capable of producing in a single process stream, through successive steps, a variety of morphologies, encompassing WS2 nanowires, a new type of 2D nanomesh morphology, and 2D in-plane mono- and few layer films. Analysis of the growth process points to two, well-decoupled stages (unlike in traditional CVD growth of 2D TMD films). One extension of the process can be seeded growth of in-plane 2D layers. A variety of techniques (i.e. transmission electron microscopy and associated analytical techniques, Raman spectroscopy, EDX, XRD, and atomic force microscopy) were used to assess the nature, composition and crystallinity of the resulting structures.

CVD growth of 2 dimensional MoS_2 and heterostructures with graphene

E Mercado[1], J Moffat[2] and R S Sundaram[1]

[1]Oxford Instruments Plasma Technology, UK, [2]Oxford Instruments Asylum Research, UK

Vapour deposition techniques have gained a lot of interest for growth of two dimensional (2D) materials[1-4]. In the recent past there has been a surge in the number of researchers studying atomic planes of other Van der Waals solids and heterostructures created by stacking layers with complementary characteristics to achieve novel functionality [5]. For successful scaling up of prototypical applications demonstrated to date, technologies and processes for large area deposition of these materials need to be developed. Here we present the technology employed and study of the impact of process parameters on a chemical vapour deposition (CVD) process for the production of single-layer MoS_2 using a gas-phase S precursor (H_2S) and solid Mo precursor ($MoCl_5$). Strategies for optimising crystalline quality via direct control of deposition variables and the impact of process parameters on defect density is analysed qualitatively using Raman spectroscopy [6]. We also present the characteristics of CVD grown MoS_2 on different substrates and investigate the use of graphene as a substrate for MoS_2 growth which opens an avenue for growth of 2D heterostructures.

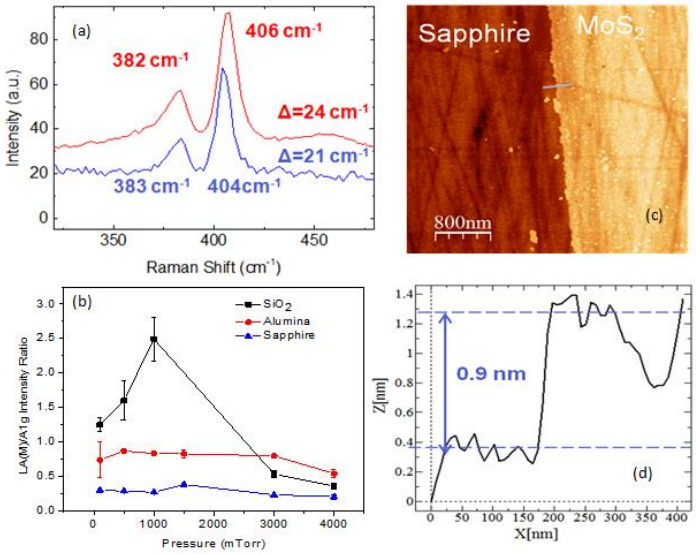

Figure1 (a) Raman spectrum of CVD deposited MoS2 (b) LA(M)/A1g peak ratio of deposited MoS2 on different substrates. (C),(d) AFM analysis of obtained films

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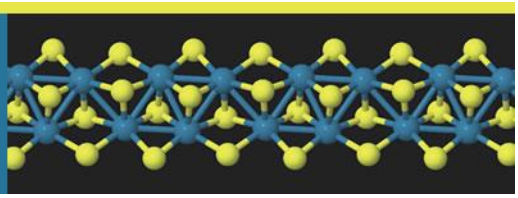
Epitaxial templating of 2D metal chlorides on monolayer MoS_2

S Wang, W Xu and J Warner

University of Oxford, UK

Developing new 2D materials beyond graphene offers the expansion of the properties of 2D systems and enhances their utility in electronics and opto-electronic applications. Monolayer transition metal dichalcogenides (TMDs), MoS_2 and WS2, are direct band gap semiconductors. Interfacing these TMDs with other 2D materials can lead to heterostructures with ideal excitonic properties for opto-electronics. I will discuss recent work on the formation of ionic metal chloride (CuCl) 2D crystals epitaxially templated on the surface of monolayer MoS_2 (figure 1). This new 2D crystal has no bulk layered form and exists purely through strong interactions with the uniform periodic surface of the MoS_2 lattice. The template, monolayer MoS_2, was grown by chemical vapour deposition (CVD) using previously reported methods[1,2] and the detailed investigations on its structural defects have been published[3]. This novel heterostructured 2D system is studied at the atomic level using aberration corrected transmission electron



microscopy at the low accelerating voltage of 80kV. Dynamics of discrete rotations of the CuCl crystal are observed, maintaining epitaxial correlations to the MoS_2 lattice directions. Strain maps are produced from displacement maps and used to track real time variations of local atomic bonding and defect production. New properties of the heterostructure system will be discussed and their potential impact on opto-electronic applications.

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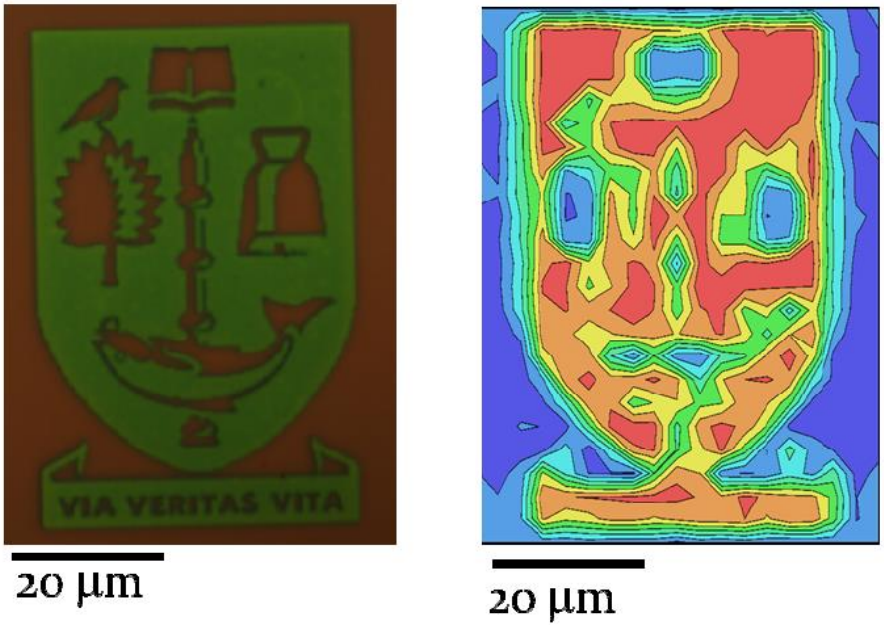
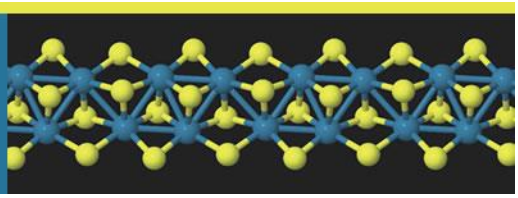
A facile topochemical route to the production of strictly 2D transition metal dichalcogenide materials

K G Crawford, S M Sivasankar, L Cosma, R Pacalaj, A Ganin and D A J Moran

The University of Glasgow, UK

Although graphene presents an attractive material solution for many electronic, optical and sensing applications, its lack of a sizeable bandgap limits its real potential for electronic device research and production. “Beyond graphene” is now the often-heard motto for the rapidly expanding advanced-functional materials research field with researchers focusing on transition metal dichalcogenide (TMD) 2D materials due to their more favourable electronic structures. For example, sizeable direct bandgap and photoluminescence in few- layered MoS_2 have already opened up the way for novel field-effect transistors and optoelectronic devices. However, the lack of a cost efficient and scalable process for large- area production of many of these materials presents a major challenge which has restricted the progress in this field from a mere scientific curiosity to a mature technology.





In this work we present a new universal method for the production of a range of 2D TMD materials which thus far we have used to demonstrate the production of MoS_2, $MoSe_2$, WS_2 and WSe_2 films on Si or Si/SiO_2 substrates. The method comprises two simple steps. The first step involves controllable growth/deposition of a thin film of transition metal oxide or transition metal on a substrate of choice using standard evaporation techniques. During the second step the film is converted into the corresponding metal sulphide or selenide using a topotactic conversion reaction. As the initial morphology and all aspects of pre-fabrication (e.g. nanopatterning) of the oxide films are preserved, this process presents a unique approach to produce well controlled, pre-patterned TMD films. The characterisation of the produced films pre and post conversion using Raman spectroscopy, X-ray diffraction, atomic force and electron microscopy are discussed in this work.

Ultrathin 2D Opto-electronics based on CVD grown crystals

H Tan, Y Fan, Y Zhou, Q Chen, W Xu and J Warner

University of Oxford, UK

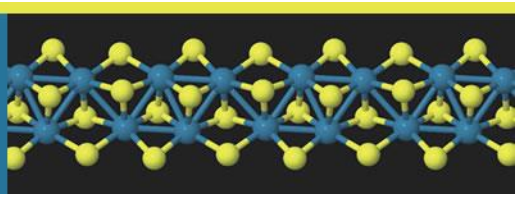
We demonstrate for the first time ultrathin (2 nm) photodetector arrays using all 2D crystals grown by chemical vapour deposition (CVD), with WS_2 monolayer as photosensitive semiconductor and graphene as electrodes. We show that graphene behaves differently to conventional metals as an electrode in photodetector due to its finite density of states associated with the Dirac cones for valence and conduction bands. The Schottky contact formed between graphene and WS_2 may thus be modified by electrostatic gating and input light control, and has led to the photodetectors' high photoresponsivity under applied gate and high illumination power. We also compare the differences between monolayer and bilayer WS_2 in photodetector applications and show that bilayer results in higher photoresponsivities due to increase photon absorption for its thicker layer number. This work of incorporating graphene electrodes in lateral TMD based devices sheds light on the contact engineering in 2D opto-electronics, which is crucial for the development of high performing ultrathin photodetector arrays for versatile applications.

In-situ atomic level observation of edge terminations of monolayer MoS_2 at elevated temperatures

Q Chen, W Xu, S Wang and J H Warner

University of Oxford, UK

Molybdenum disulfide (MoS_2) is a widely explored transition metal chalcogenide, which has attracted massive interests over the last decade for various next-generation electrical and optoelectronic device applications. To thoroughly understand the behaviours in its concurrent use, and exploit new applications, structural study for monolayer MoS_2 with atomic resolution is indispensable. Aberration corrected transmission electron microscopy (AC-TEM) is a powerful tool for observation of atomic structure with single atom sensitivity, and when combining with in-situ heating holder, the structures can be imaged up to 800°C, which provides us an opportunity to explore the structural change during heating process. Here we report the edge terminations of MoS_2 at 800°C with atomic resolution. Without the interference of crystallized carbon films, which is ubiquitous at low temperatures induced by the electron beam, the edge terminations at elevated temperatures are sharp and neat. Several types of edge configurations has been observed, which are entirely different from the structures at room temperature. These observations shed light on the high-temperature applications, including electronics and sensors, as well as targeted design for nanopores within monolayer MoS_2 for water desalination and nanopore-based DNA sequencing.



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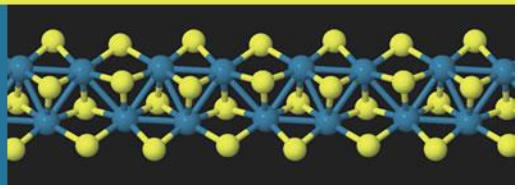

Friday 2 September

(Invited) Photonics and polaritonics with van der Waals heterostructures

A I Tartakovskii

University of Sheffield, UK

Monolayer films of van der Waals crystals of transition metal dichalcogenides (TMDCs) are direct band gap semiconductors exhibiting excitons with very large binding energies and small Bohr radii, leading to a high oscillator strength of the exciton optical transition. Together with graphene as transparent electrode and hexagonal boron nitride (hBN) as an insulator, TMDC monolayers can be used to produce so-called van der Waals heterostructures. Here we use this approach to make electrically pumped light-emitting quantum wells (LEQWs) and single-photon emitters. We combine this new technology with optical microcavities to demonstrate control of the emitter spectral properties and directionality, making first steps towards electrically injected TMDC lasers. Furthermore, by embedding $MoSe_2$/hBN structures in tuneable microcavities, we enter the regime of the strong light-matter interaction and observe formation of exciton-polaritons. Furthermore, we demonstrate that the magnitude of the characteristic anti-crossing between the cavity modes and the $MoSe_2$ excitons (a Rabi splitting) can be enhanced by embedding a multiple-QW structure, containing two $MoSe_2$ monolayers separated by an hBN barrier. At a temperature of 4K, for a single QW sample the vacuum Rabi splitting of 20 meV is observed for the neutral exciton state, which is increased to 29 meV for the double QW, following closely the $\sqrt{N_{QW}}$ dependence. An intermediate coupling regime is observed for the charged exciton, where the polariton states are not fully resolved as the Rabi splitting is similar to the charged exciton linewidth. We extend this work to demonstrate valley addressable polaritons in both $MoSe_2$ and WSe_2, the property inherited from valley excitons, but strongly modified through changes in exciton relaxation in the strong-coupling regime. This work opens a new avenue in the field of polaritonics in a new material system of van der Waals crystals and heterostructures with a potential for polariton devices operating at room temperature.

Interlayer excitons in van der Waals heterostructures

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[1]University of Sheffield, UK, [2]The University of Manchester, UK

Recent success in producing vertical stacks of different two-dimensional (2D) materials has enabled development of novel devices based on van der Waals heterostructures (HSs) [1]. Properties of such HSs can be suitably tuned by incorporating monolayers of semiconducting transition metal dichalcogenides (TMDs) having direct bandgaps [2] and large exciton binding energy [3-5]. The presence of long-lived interlayer excitons (IXs) in HSs with type-II band alignment (Fig. 1(a)) has been recently demonstrated [6].

In our work, we investigate IXs in $MoSe_2$-WSe_2 HSs using photoluminescence excitation and polarisation-resolved photoluminescence (PL) spectroscopy. We demonstrate that their binding energy and PL intensity can be highly tuned by electrostatic gating (Fig. 1(c)). The IX PL signal exhibits a blueshift with increasing laser excitation power (Fig. 1(d)), occurring due to repulsive interaction between IXs [7]. The unique properties of IXs open new ways to explore many-body physics in TMDs, which otherwise are only accessible at very high exciton densities due to small exciton radii in these materials.

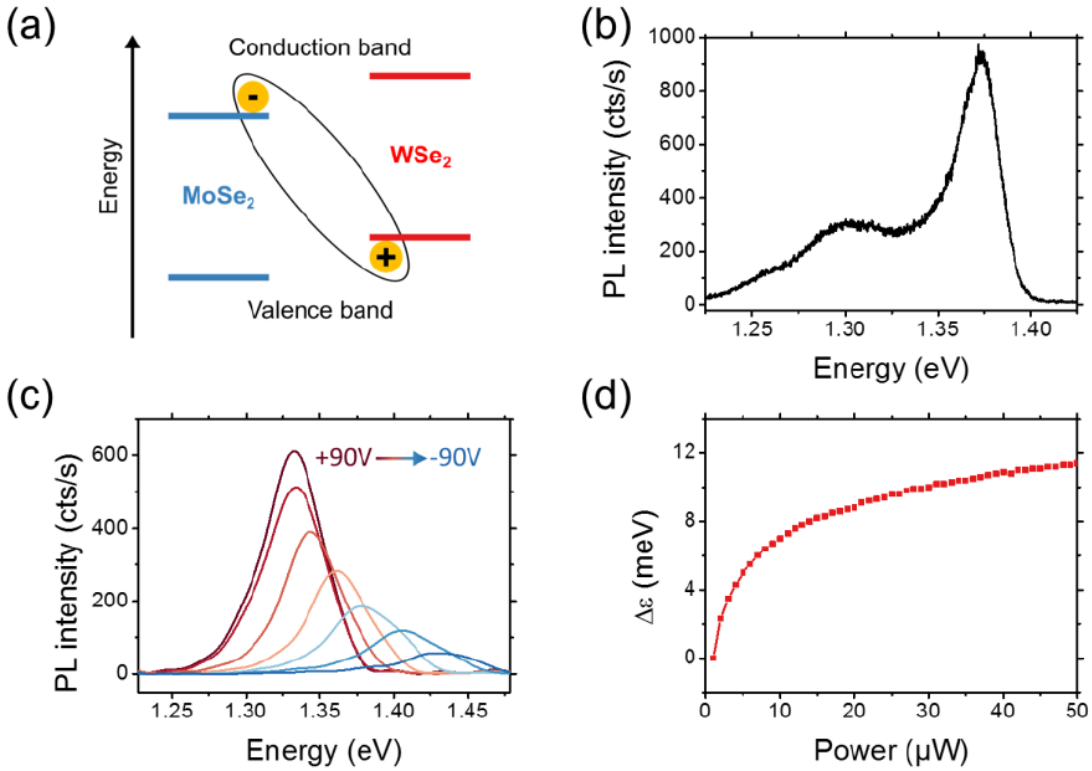

Fig. 1. (a) Schematics of band alignment in $MoSe_2$-WSe_2 HS. (b) IX PL signal from HS for laser excitation power 20 μW and temperature 8 K. (c) IX PL spectrum as a function of applied gate voltage. (d) IX peak position change Δ as a function of excitation power.

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Large scale CVD 2D heterostructures

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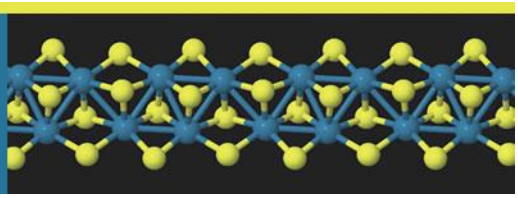
University of Southampton, UK

Currently, 2D Transition metal dichalchogenides are emerging as the next generation semiconductor materials as they offer a direct bangap and therefore high on/off ratios, relatively high mobility, short-channel effects immunity, and near ideal subthreshold swings [1, 2]. We have previously reported a technology that enables us to grow MoS2 thin films and monolayers directly on a variety of substrates by atmospheric pressure chemical vapor deposition (APCVD) at ambient temperature followed by a two-step annealing process [3]. This process uses industry standard equipment and is scalable. Both of which aspects constitute it an excellent candidate for the realization of large scale complementary structures for high performance electronic applications.



In this work we present an expanded version of our APCVD process which enables us to create 2D heterostructures such as diodes and gates. The process results in vertical junctions and involves the growth of MoS_2 as the n-type and $MoSe_2$ as the p-type semiconductor on SiO_2 coated wafers. The first step involves the patterning of an AZ2070 negative resist layer which is followed by the room temperature deposition of a Mo-S film using MoCl5 and H_2S as the precursors. The low temperature allows the survival of the photoresist, the use of which makes the process simpler. The H_2S is introduced in saturation so that the resulting film stoichiometry is that of an amorphous MoS3 layer. After deposition the photoresist is lifted-off to leave the desired patterns on the wafer. This process is then repeated to create an overlapping amorphous $MoSe_2$ layer using MoCl5 and Se as precursors .The last step of the process is the crystallization annealing of the deposited materials. To electrically contact the two materials metal contacts are formed by sputtering a Ti/Au layer in a lift-off process. Finally, a dielectric capping layer is formed over the semiconducting films by sputtering HfO_2.

The resulting films where characterized by SEM, Raman, and XPS. The SEM showed the successful deposition of a-few-layers for both materials which was confirmed by comparing the characteristic Raman peak separation for the two materials. The magnitude of the Raman peaks were used to verify the high crystallinity of both materials. The use of XPS was imperative as it revealed that the films were successfully reduced to MoS_2 and $MoSe_2$. To demonstrate the viability of the process we fabricated single doping n- and p-type transistors and pn-junction diodes on the same wafer. The electrical characterization of these devices will enable us to further optimize and improve the process, to enhance the electrical performance, but also demonstrate devices with more complicated geometries such as npn transistors.

The significance of this technology lies within the simplicity and the low-step count. By employing the low temperature APCVD it was possible to use a lift-off resist for the patterning, eliminating the need for a hard (oxide) mask layer [4]. Our process works for wafer scale processing and results in an increased yield. The vertical junctions can be used to create devices such as atomically thin diodes and high performance 2D complementary transistors in a large scale. As a result it brings the inclusion of 2D semiconductors in commercial electronics closer. Finally, it opens up capabilities towards the realization of high performance devices such as 2D tunneling transistors that will enable sub-60 mV/dec subthreshold slopes to substantially increase power efficiency.

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Resonantly excited exciton dynamics in two-dimensional MoSe2 layers

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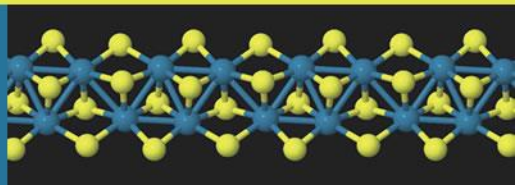
Single layers (SL) of transition-metal dichalcogenide (TMD) are of significant interest both for fundamental physics and their possible application in optoelectronics and photovoltaics. They have a direct bandgap, with the conduction and valence band extrema (valley) at the corners (+K and -K point) of the hexagonal Brillouin zone [1]. Due to spin-orbit interaction and the missing inversion symmetry, the electron and hole valley (±K) and spin are linked to the circular polarization direction of the optical transition [2]. This leads to valley-dependent optical selection rules, giving TMDs unique properties for optoelectronic devices. We performed resonant three-pulses four



wave mixing (FWM) spectroscopy as function of temperature (300-77 K) on a SL of MoSe2. The FWM is measured in phase and amplitude by heterodyne detection [3], with a time resolution given by the field autocorrelation of the pulse (200 fs). By performing a complex multi- exponential fit to the data we extracted the timescales as well as the relative phases of the processes involved in the exciton dynamics. Measurements of the A-exciton density decay show three well-defined timescales of the order of 0.1 ps, 10 ps and 100 ps, respectively. An additional timescale of 1-100 ns, longer than the pulse repetition period of 12 ns is also found. The first timescale decreases with the excitation power and is attributed to radiative recombination and exciton-exciton scattering. The presence of the longer timescales shows that excitons also populate dark states that have different decay times. Temperature dependent measurements clearly demonstrate that exciton-phonon scattering is the main mechanism that populates dark states. We interpret the data considering dark states of the intrinsic band structure of SL-TMD, without resorting to extrinsic effects. We also show that exciton-exciton annihilation is not relevant to describe the observed dynamics. Exciting resonantly the trion transition, the initial decay is longer, whereas the later dynamics is similar, as expected from the longer radiative lifetime and the thermalisation with excitons on longer timescales.

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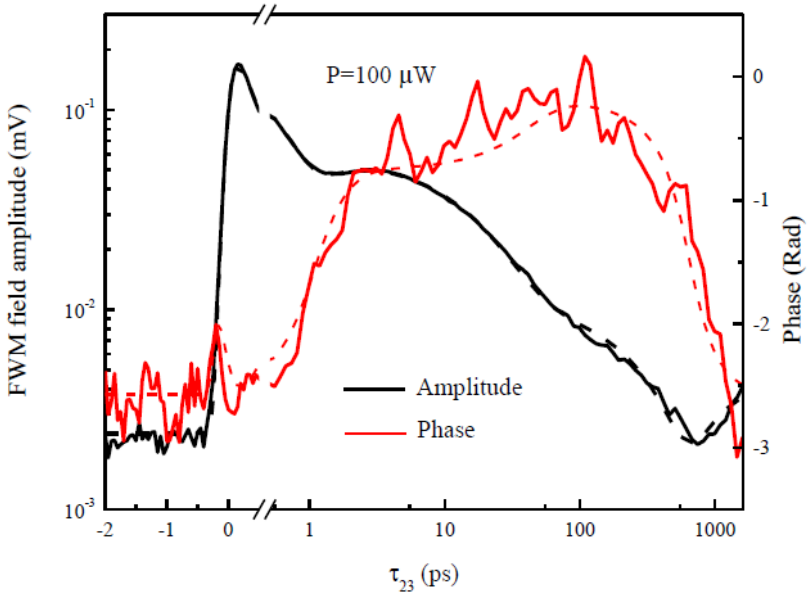

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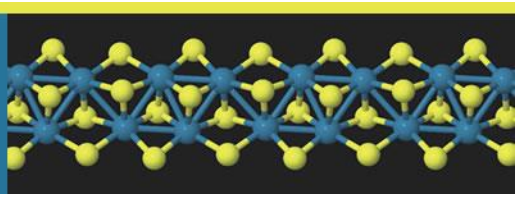
1–2 September 2016, University of Bath, Bath, UK



Deterministic localisation and resonant laser spectroscopy of quantum emitters in mono- and bi-layer WSe_2

A Branny[1], S Kumar[1], M Brotons-Gisbert[2], R Al-Khuzheyri[1], G Ballesteros-Garcia[1], J F Sánchez-Royo[2] and B D Gerardot[1]

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Two-dimensional (2D) semiconductors such as transition metal dichalcogenides (TMDs) which can host quantum emitters[1] have recently emerged as a new platform for quantum photonics. 2D materials are intriguing solid-state systems due to their unique relation to uniform strain[2,3]. In localised form, strain is responsible for the exciton funnel effect[4] and was shown to induce the localisation and shift the emission energy of quantum emitters in WSe_2[5]. Here we exploit pre-patterned substrates as a strain engineering technique to tackle the random distribution of single photon sources present in TMDs. We demonstrate that localized strain provides sufficient change in the local electronic bandgap to spatially trap carriers. This scheme reliably yields spectrally clean, spatially and spectrally isolated quantum emitters at pre-defined locations. We observe high purity single photon emission from pre-defined sites. This approach simplifies future spectroscopy and characterization of the nature of the quantum emitters and opens a path towards integrated photonics with TMD based quantum emitters. Moreover, we perform resonance and near-resonance excitation of isolated quantum emitters to reveal near ideal single photon fluorescence and uncover weakly-fluorescent exciton states ~ 5meV blue-shifted from the bright exciton states[6]. Resonance fluorescence and high single photon purity demonstrate the potential for coherent quantum optics in such emitters.

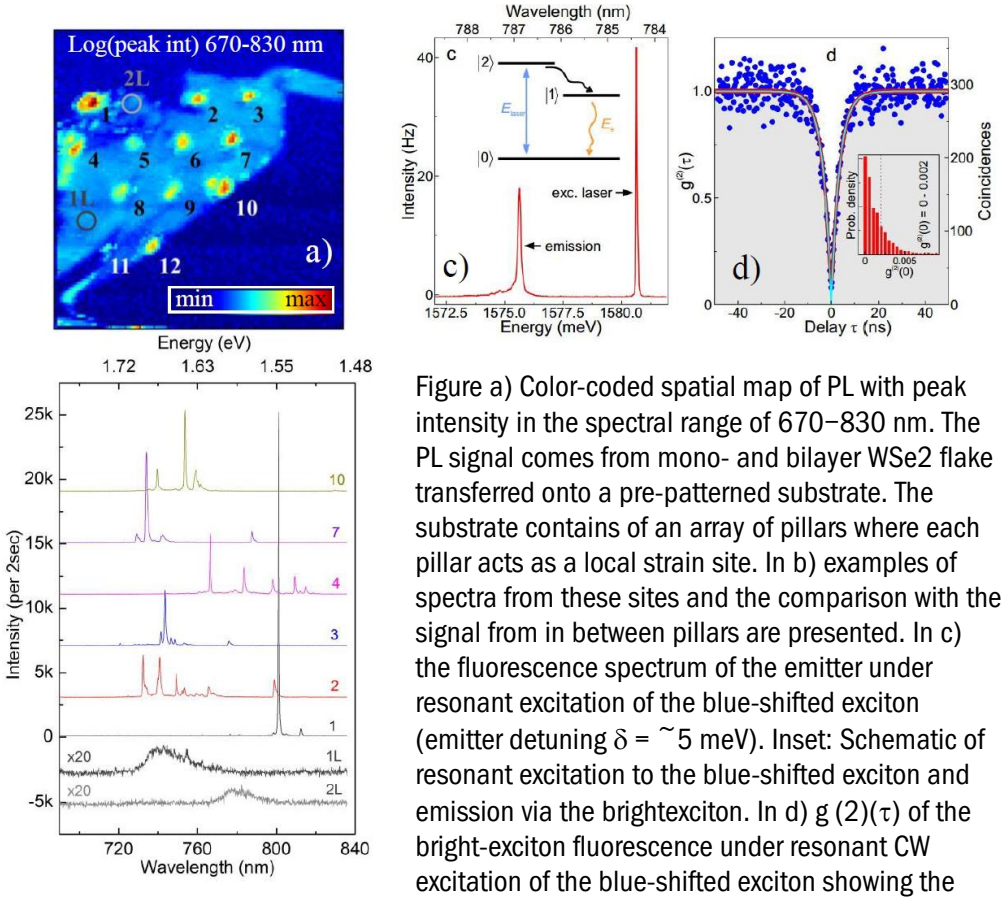
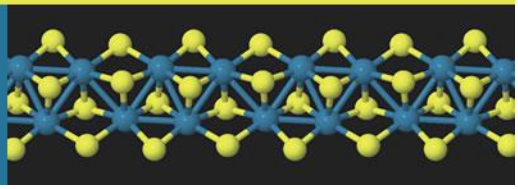


Figure a) Color-coded spatial map of PL with peak intensity in the spectral range of 670–830 nm. The PL signal comes from mono- and bilayer WSe2 flake transferred onto a pre-patterned substrate. The substrate contains of an array of pillars where each pillar acts as a local strain site. In b) examples of spectra from these sites and the comparison with the signal from in between pillars are presented. In c) the fluorescence spectrum of the emitter under resonant excitation of the blue-shifted exciton (emitter detuning δ = ~5 meV). Inset: Schematic of resonant excitation to the blue-shifted exciton and emission via the brightexciton. In d) g (2)(τ) of the bright-exciton fluorescence under resonant CW excitation of the blue-shifted exciton showing the high purity single photon emission.



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Room temperature Tamm-Plasmon Exciton-Polaritons with a WSe_2 monolayer

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We discuss the observation of Tamm-Plasmon Exciton-Polaritons with a WSe_2 monolayer at room temperature. The high thermal stability and large oscillator strength of excitons in monolayers of transition metal dichalcogenides make them ideal candidates for room temperature polaritonics. Recently, photoluminescence emission in the strong coupling regime was reported for a $MoSe_2$ monolayer at 4 K [1]. Compared to $MoSe_2$, WSe_2 monolayers exhibit a strongly enhanced photoluminescence (PL) yield at room temperature and a significantly narrower PL emission linewidth compared to MoS_2 [2]. We thus embedded a WSe_2 monolayer in a compact Tamm structure, which consists of a distributed Bragg reflector, onto which the monolayer was exfoliated. The monolayer was capped by a layer of poly(methyl methacrylate) and the device was completed by a gold layer. This photonic micro-structure provides the very small mode volume which enhances light matter coupling.

In such a device, we confirmed strong coupling conditions at ambient conditions, and mapped out the characteristic exciton-polariton dispersion relation by in-plane momentum-resolved PL spectroscopy. Figure 1a shows the PL spectra for various in-plane momenta. Fitting the peak energies allows to plot the full dispersion relation presented in figure 1b (symbols). The acquired dispersion relations can be well fitted with a coupled-oscillator model (solid lines in figure 1b) featuring a Rabi splitting of 23.5 meV and a distinct potential minimum at zero momentum. Moreover, we discuss a theoretical model for the population of the polariton states, assuming a Boltzmann distribution with a temperature of 300 K, which shows excellent agreement with the experimental results [3].

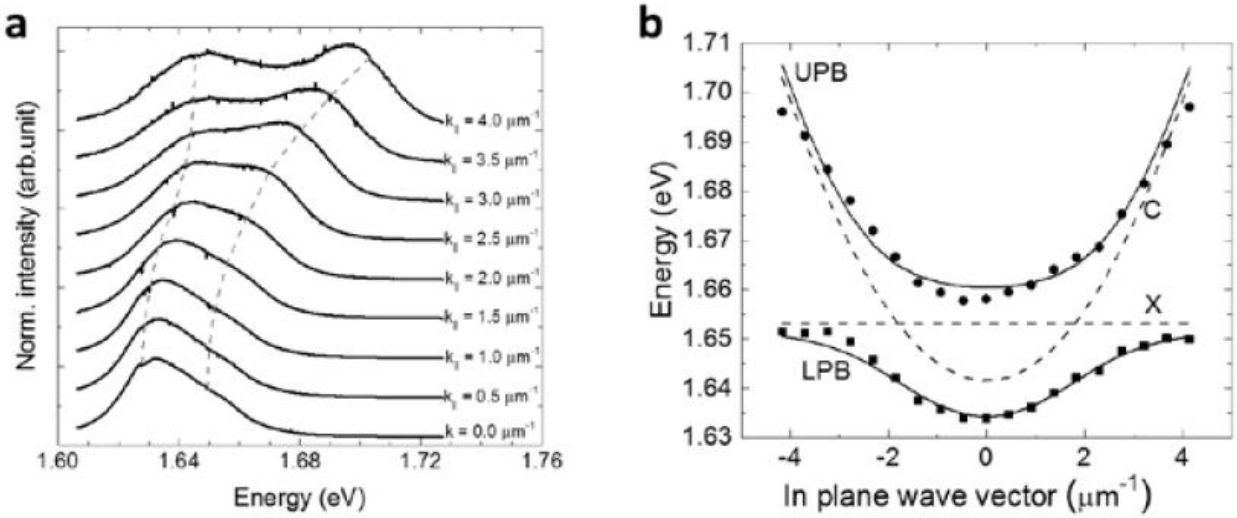

Fig. 1. a, PL spectra at various in-plane momenta. b, Polariton dispersion relations at 300 K.

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(Invited) Direct k-space imaging of spin-valley locking in transitionmetal dichalcogenide semiconductors and superconductors

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University of St Andrews, UK

A locking of the spin with the valley degree of freedom [1] is one of the defining properties of monolayer transition-metal dichalcogenide (TMD) semiconductors such as MoS_2 and WSe_2, leading to a range of exciting optoelectronic properties such as chiral light emission and a valley Hall effect [2,3]. Here, we will report the direct momentumspace imaging of such spin-valley locking in TMDs via spin- and angle-resolved photoemission spectroscopy. We will show how spin-valley locking is not restricted to monolayer TMDs, but persists in bulk systems, with the spin additionally becoming locked to the layer pseudospin. Our direct observation of spin-polarised valence bands in 2H-WSe_2 is in contrast to conventional expectations for this non-magnetic and centrosymmetric system, and points to a new route to stabilize "hidden" spin textures in solids driven by local inversion asymmetry. We will show how control of the layer degeneracy via chemical gating (analogous to field-effect doping) leads to large and highly tuneable valence band spin splittings [5], as well as a surprisingly large influence of many-body interactions due to weak screening of Coulomb interactions in the resulting multi-valley 2DEG that forms. We will also show how spin-valley locking persists in other transition-metal dichalcogenides, including the well-studied charge-density wave and superconducting system 2H-$NbSe_2$ [6]. Here, increased interlayer interactions cause a particularly rich three-dimensional momentum-dependent spin texture to develop, necessitating a fundamental reconsideration of charge order and superconductivity in this and related systems.

[1] Xiao et al., Phys. Rev. Lett. 108 (2012) 196802
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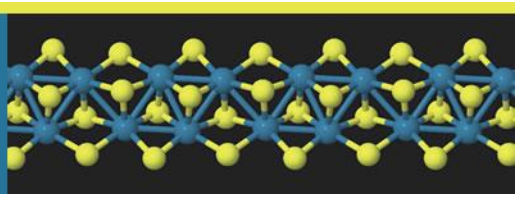

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Direct determination of band offsets, hybridization and exciton binding in 2D semiconductor heterostructures

N R Wilson[1], P V Nguyen[2], K Seyler[2], P Rivera[2], A J Marsden[1], Z P L Laker[1], G C Constantinescu[3], V Kandyba[4], A Barinov[4], N D M Hine[1], X Xu,[2,5] and D H Cobden[2]

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Combining monolayers of different two-dimensional (2D) semiconductors into heterostructures opens up a wealth of possibilities for novel electronic and optical functionalities. Exploiting them hinges on accurate measurements of the band parameters and orbital hybridization in separate and stacked monolayers, many of which are only available as small samples. The recently introduced technique of angle-resolved photoemission spectroscopy with submicron spatial resolution microARPES) offers the capability to measure such small samples. Here, we show that by suitable heterostructure sample design the full potential of microARPES can be realized, revealing full valence band parameters of micron scale flakes of 2D materials with energy resolution of ~ 50 meV. This simply demonstrates the evolution of bandstructure with layer number, but here we focus on $MoSe_2/WSe_2$ van der Waals heterostructures, which are 2D analogs of 3D semiconductor heterostructures. We find that in a $MoSe_2/WSe_2$ heterobilayer the bands in the K valleys are weakly hybridized, with the conduction and valence band edges originating in the $MoSe_2$ and WSe_2 respectively. There is stronger hybridization at the Γ point, but the valence band edge remains at the K points. This is consistent with the recent observation of interlayer excitons where the electron and hole are valley polarized but in opposite layers. We determine the valence band offset to be 300 meV, which combined with photoluminescence measurements, implies that the binding energy of interlayer excitons is at least 200 meV, comparable with that of intralayer excitons. These results directly answer many outstanding questions about the electronic nature of $MoSe_2$-WSe_2 heterobilayers, and demonstrate the efficacy of spatially resolved ARPES in probing device-scale structures of 2DM.

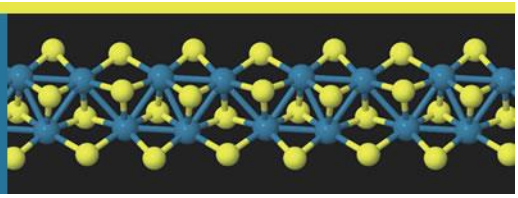
Linear-scaling DFT simulations of layered material heterostructures

N D M Hine[1], N Yeung[1] and G C Constantinescu[2]

[1]University of Warwick, UK, [2]University of Cambridge, UK

Layered material heterostructures enable us to combine favourable electronic and optical properties of individual layered materials, such as transition metal dichalcogenides, in almost any combination by appropriate stacking and stitching. Such structures have applications to low-power electronics, optoelectronics, photovoltaics and many other fields. As the constituents of these electronic devices become ever smaller, the need to incorporate accurate quantum mechanical simulations into device design becomes increasingly pressing. We present several projects harnessing the power of high accuracy linear-scaling density functional theory calculations using the ONETEP LS-DFT code, to understand the properties of these materials and simulate realistic device architectures [2-4].

I will introduce the capabilities of the code, including Projector Augmented Wave methods and nonlocal van-der-Waals functionals. Using large simulation cells we can explore possible constructions of layered material



heterostructure interfaces. We can vary rotation, translation and separation of multiple vertically-stacked layers without introducing unrealistic strain. The resulting energy landscape shows that the constituents are essentially energetically invariant under rotation, with no strongly-preferred alignments. We can also simulate device performance, such as for tunnelling Field Effect Transistor applications [2]. By simulating ARPES measurements, we show that the electronic bandstructures of each layer are coupled by interlayer hybridisation, such that band offsets and effective masses can be altered, significantly affecting electronic and optical properties[3]. In combination with experimental ARPES measurements, we have been able to demonstrate the coexistence of aligned and misaligned regions in lattice-matched, nearly-aligned vertical heterostructures [4]. Finally I will introduce ongoing work on lateral heterostructures, particularly in relation to defect segregation.

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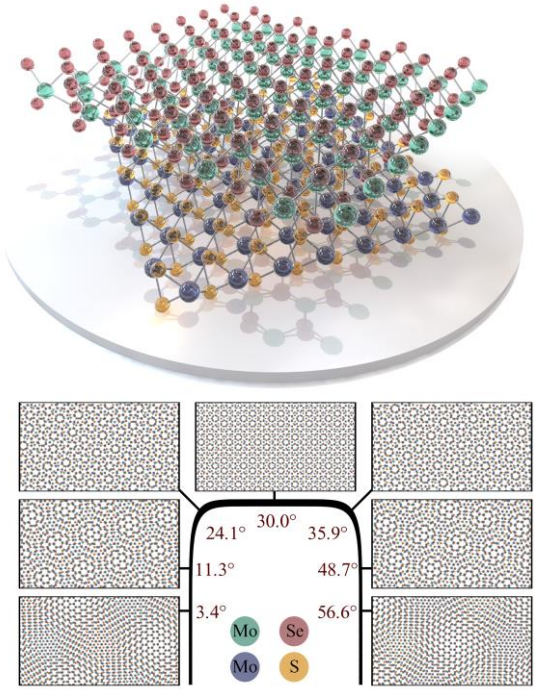
Band-structure effects in vertical layered-material heterostructures

G Constantinescu[1] and N Hine[2]

[1]University of Cambridge, UK, [2]University of Warwick, UK

While monolayer forms of 2D materials are very well-characterised both experimentally and theoretically, properties of vertical heterostructures are not nearly so well-known. We employ high-accuracy linear-scaling DFT calculations to explore large-scale models of transition metal dichalcogenide and hBN/Phosphorene heterostructures. Band modifications upon stacking and rotation of different monolayers can be obtained by unfolding the supercell spectral function into the primitive cells, allowing direct comparison to experimental ARPES results. Changes in spectral weight and band-structure between the monolayers and heterostructured interfaces show how lattice mismatch (TMDC/TMDC) or spacer layers (Phosphorene/hBN/Phosphorene) allow the component monolayers to retain more independence in heterostructures than in homo-stacks. Moreover, one can envision using cavities in spacer layers in order to confine the radial extent of a vertical heterostructure, with potential applications in optoelectronics.



Suppression of inter-valley relaxation in monolayer WSe_2 with small magnetic fields

T P Lyons[1], S Dufferwiel[1], S Schwarz[1], F Withers[2], K S Novoselov[2], and A I Tartakovskii[1]

[1]University of Sheffield, UK, [2]University of Manchester, UK

In monolayers of WSe_2, bright excitonic species have been shown to exhibit strong chiral selectivity owing to the locking of light helicity to the valley degree of freedom [1,2]. The degree of valley initialisation that can be achieved is limited by inter-valley scattering of excitons due to the strong electron-hole exchange interaction which has been shown to be a significant, although inefficient, mechanism for valley pseudo-spin relaxation [3]. Here we study the magneto-PL dependence of a van der Waals (VDW) heterostructure consisting of a WSe_2 flake encapsulated with thin films of hBN, as shown in Fig.1a. PL-spectra from the sample, shown in Fig. 1b, exhibit strong excitonic features associated with the neutral (X0), charged (X-) and localised (P1) excitons along with a band of localised emitters (LEs). We demonstrate that the application of a small magnetic field in Faraday geometry ($B < 500mT$) leads to a large increase in X- and P1 valley polarisation of $\sim 40\%$ of its zero field value, which we attribute to suppression of intervalley relaxation (Fig. 1c). Furthermore, a clear transition to Hanlé-like depolarisation behaviour is observed in both the trion and localised emitter band as the applied external B-field is tilted from Faraday to Voigt geometry, as shown in Fig. 1d. In addition to this work, the narrow linewidths displayed by our WSe_2 samples have allowed observation of an in-plane field dependent valley splitting and associated g-factor of -1.8. This demonstration of significant suppression of pseudo-spin relaxation opens new possibilities for engineering valley relaxation channels through the use of VDW heterostructures in small magnetic fields.

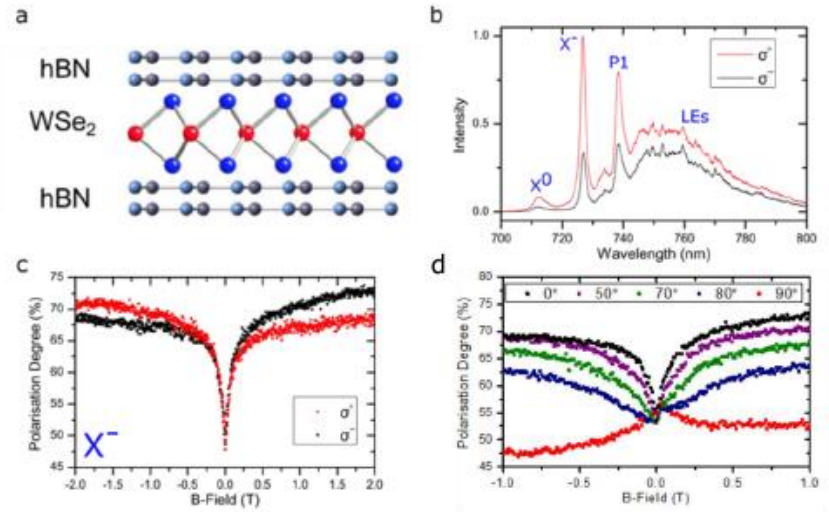


Fig.1. **a** Schematic of the van der Waals heterostructure. **b** PL spectra under σ+ polarized excitation at 637 nm with collection co- and cross-polarized. c, d Degree of polarisation for X- as a function of magnetic field in c, Faraday geometry and d, fields applied at various angles from Faraday (0˚) to Voigt (90˚, in-plane) geometries.

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Cavity enhanced light extraction from monolayer topological defects

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The integration of two-dimensional transition metal dichalcogenides (TMDs) with nanoscale photonic structures, such as photonic crystal cavities [1] have recently emerged as a promising approach towards on-chip opto-electronic devices. Here we demonstrate a design of silicon photonic crystal [2], consisting of nano-rods arranged in a triangular lattice, with a defective cavity. The curvature of the monolayer suspended over the cavity induces lateral stress, which can promote the formation of topological defects close to the curvature minimum. We tuned the cavity to resonate with the emission wavelength of MoS_2 and showed substantial improvement to the overall optical efficiency. This result will allow topological defects in TMDs to be investigated under the light of a resonant cavity.

Existing implementations of cavity controlled emission take advantage of slab photonic crystals, where vertical mode loss is minimised. However, spatial coupling between the cavity field maximum and the optically created excitons is limited due to geometry. Furthermore, monolayers transferred onto substrates using mechanical exfoliation or otherwise tend to have topological defects, including ripples, curvature and folds [3], further limiting the spatial coupling. We consider the alternative, where silicon nano-rods arranged in a triangular lattice provide both spectral and spatial coupling between the monolayer TMD and the cavity mode, due to the natural curvature of the suspended monolayer. We find up to 350% enhancement of collected power from cavity coupled emission, over a monolayer exfoliated on a flat substrate.

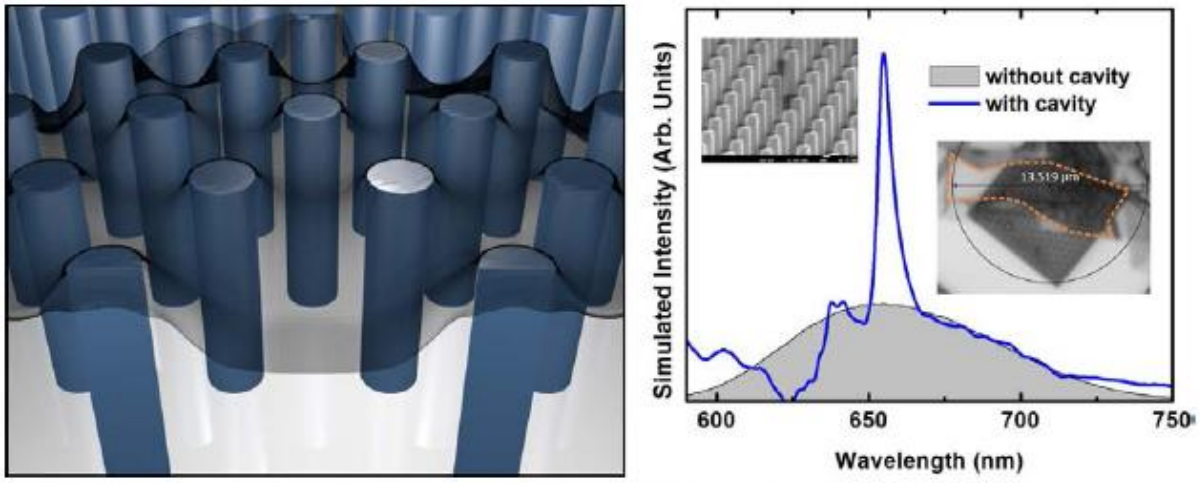

Figure 1: (Left) Illustration of nano-rods with a suspended monolayer. (Right) Simulated spectra from a monolayer suspended over a cavity and one on silicon/silicon dioxide substrate. Insets show the scanning electron micrograph of the nano-rods and an optical image of a MoS_2 flake transferred on top of a photonic crystal cavity, orange outline indicate the transferred flake.

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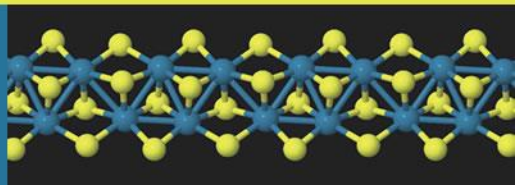
3D printing of MoS_2 nanosheets

C Grotta and C Mattevi

Imperial College London, UK

Atomically thin metal VI- dichalcogenides (TMDs) have attracted increasing attention in the last few years thanks to their complementary properties to graphene. The atomic thickness, optoelectronic properties, mechanical flexibility and specific surface area are among the most remarkable characteristics of monolayer VI-metals dichalcogenides. Their properties can be further exploited if the flakes can be arranged to form a three-dimensional (3D) network with tailored mechanical properties and specific surface area. Group VI- TMDs constructs could see applications ranging from energy conversion to bioelectronics. We report fabrication of 3D printable inks of cross-linked MoS_2 flakes in biocompatible polymers. MoS_2 bulk powders are chemically exfoliated in aqueous suspensions to obtain nanosheets with 1T and 2H atomic coordination and subsequently are cross-linked with a class of three blocks copolymers. The polymers analysed behave as amphiphilic molecules, and are thermo responsive, allowing the formation of a gel-ink. The chosen three block polymers have hydrophilic and hydrophobic groups, enabling homogenous dispersion of the nanosheets in water. The inks are 3D printed via robocasting to form selfsupporting 3D macroscopic structures of exfoliated MoS_2 nanosheets. The specific surface area, mechanical properties and electrical conductivity of the 3D printed structures are systematically studied in the context of different applications. We further demonstrate that the introduction of additives in the inks can impart different functionalities.



Poster abstract

P.1 Optoelectronic properties study of atomically thin ReSSe with weak interlayer coupling

V Zólyomi[1], F Liu[2], S Zheng[2], A Chaturvedi[2], J Zhou[2], Q Fu[2], C Zhu[2], P Yu[2], Q Zeng[2], N D Drummond[3], H J Fan[2], C Kloc[2], V I Fal'ko[1], X He[2] and Z Liu[2]

[1]The University of Manchester, UK, [2]Nanyang Technological University, Singapore, [3]Lancaster University, UK

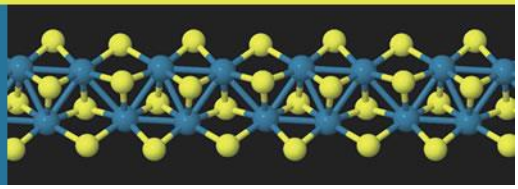
Rhenium dichalcogenides, such as ReS_2 and $ReSe_2$, have attracted a lot of interests due to the weak interlayered coupling in these materials. Studies of rhenium based dichalcogenide alloys will help us understand the differences between each binary rhenium dichalcogenides. They will also extend the applications of two-dimensional (2D) materials through alloying. In this work, we studied the optoelectronic properties of ReSSe with S and Se ratio of 1:1. The band gap of ReSSe alloy is investigated by optical absorption spectra as well as theoretical calculations. The alloy shows weak interlayered coupling, as evidenced by the Raman spectrum. A field-effect transistor based on ReSSe shows typical n-type behaviour with a mobility of about 3 $cm^2V^{-1}s^{-1}$ and an on/off ratio of 10^5, together with the in-plane anisotropic conductivity. The device also shows good photoresponse properties, with a photoresponsivity of 8 A/W. The results demonstrated here will provide new avenues for the study of 2D materials with weak interlayer interactions and in-plane anisotropy (F. Liu et al, Nanoscale 8, 5826 (2016)).

P.2 Uniform growth of a wafer scale MoS_2 monolayer using chemical vapor deposition (CVD)

O Omar and Y Jun

University of York, UK

Monolayer Molybdenum disulfide (MoS_2), a two dimensional semiconductor with direct band gap of 1.9 eV, has been proposed as a candidate for the next generation Nano electronic and optoelectronic devices. As in the case of graphene, initial work was carried out on MoS_2 started by mechanical exfoliation which can produce high quality MoS_2 monolayers. However due to the low production rate, this technique is limited to the research purpose. For practical application, mass production techniques must be developed [1, 2]. The growth of large area MoS_2 has been reported using CVD based techniques. The sulfurization of pre-deposited Mo metal or Mo oxides can produce large area of MoS_2, however this approach produce spatially inhomogeneous MoS2 layers [3, 4]. Molybdenum pentachloride ($MoCl_5$) a reasonable precursor to be used in the CVD to achieve better thickness control, but due to the toxicity of $MoCl_5$, a special care is needed during the growth [5]. The metalorganic CVD is also another option to deposited large MoS_2 area, however the grains produced has been very small in size (about 2 μm) and the growth is time consuming about (26 hour) for each growth run [6]. In this work molybdenum dioxide (MoO_2) and sulfur powders are used to grow MoS_2 mono layers at elevated temperatures T≥800 °C. A careful optimization of growth parameters such as temperature, pressure and precursors amounts led to growth in a uniform wafer scale (up to 5 cm, the size is limited to our tube furnace) with grain size up to 400 μm. The uniformity of the monolayer film is confirmed using second harmonic generation microscopy SHG. The monolayer MoS_2 was characterized using atomic force microscopy (AFM), Raman spectroscopy, Second harmonic generation SHG, photoluminescence (PL) spectroscopy, x-ray photoemission spectroscopy (XPS), and transmission electron microscopy (TEM). The advantage of our approach is not only because of the large area high quality films with large domain size one can produce, but also the procedure is potentially less hazardous than other methods tried as well as short period growth time (about only 15 minuet) for each growth run.



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P.3 ARPES study of intercalated bulk MoS_2 superconductors

M B Subhan[1], M Watson[2], Z Liu[3], A Walters[2], M Hoesch[2] and C Howard[1]

[1]University College London, UK, [2]Diamond Light Source, UK, [3]ShanghaiTech University, China

Transition-metal dichalcogenides (TMDCs) are a group of layered materials that exhibit a rich array of electronic ground states including semiconductivity, metallicity, superconductivity and charge density waves (CDW)[1]. In recent years the ability to isolate and study individual layers, for example, by incorporation into nanoscale devices, has reinvigorated research into these materials.

It has been shown that the charge carrier density (electron doping) in few layer MoS_2 can be tunably increased via electrostatic gating[2]. Interestingly, at high doping MoS_2 exhibits superconductivity, with a “dome-like” dependence of T_c on doping analogous to that found in the cuprate superconductors[2]. The high doping required for superconductivity can also be achieved via intercalation of alkali metals in the van der Waals gaps of bulk MoS_2[3,4]. In both the few layer and bulk cases the origin of this superconductivity is not yet understood with predictions ranging from exotic pairing mechanisms in bulk systems[5,6,7] to Ising superconductivity in single layers8,9,10. Investigating the bulk doped compound permits experimental interrogations of these phenomena, not possible in a gated nanodevice environment.

In this poster we present our work on MoS_2 intercalated with alkali metals using a low temperature metal ammonia solution[3]. X-ray diffraction measures an increase in the layer separation for all intercalated samples, as well as 2x2 superstructure formed by the potassium ions in $K_{0.4}MoS_2$. ARPES data reveals the electronic structure of superconducting intercalated MoS_2 including the first measurement of electron pockets at the Fermi surface of $K_{0.4}MoS_2$ which is consistent with a 2 x 2 zone folding lattice.

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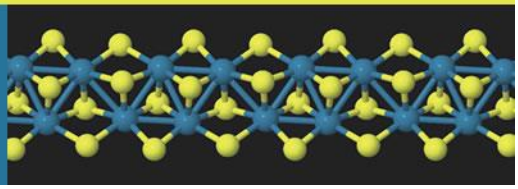

P.4 Tuning correlated electron states in few-layer 2H-TaS2 by field-effect gating

H Shajari, S Dale, D Wolverson and S J Bending

University of Bath, UK

Van der Waals bonded layered compounds such as transition metal dichalcogenides (TMDs) have recently attracted renewed interest due to electronic instabilities arising as a result of their two dimensional nature, e.g., charge density waves (CDWs) and superconductivity. TaS_2 is one such layered material, which exhibits charge density wave states that are believed to compete with superconductivity. We describe investigations of the temperature-dependent electrical properties of few-layer 2H-TaS_2 samples as a function of electrostatic gating. Micromechanical exfoliation was used to produce high quality single-crystal few molecular layer TaS_2 flakes on Si/SiO_2 (300 nm) substrates. AFM and Raman Spectroscopy of few-layered and 'bulk' 2H-TaS_2 has been performed and characteristic Raman peaks were observed in thick flakes of 2H-TaS_2 at 400 and 301.5 cm^{-1}. Flakes were then patterned using electron beam lithography and Cr/Au contacts evaporated for use as the channel of field effect transistors (FETs). The highly doped Si substrate can be used as a back gate to vary the carrier concentration in the channel and an integrated 'top gate' allows use with ionic liquids. TaS_2 has three common polytypes, 1T, 2H and 3R, while at ambient conditions only 2H-TaS2 undergoes both a superconducting transition at 0.8 K and a CDW transition at 70 K in bulk samples[1,2]. In 10nm thick 2H-TaS_2 flakes, we show that the resistive signature of a CDW is still observed, but at the slightly higher onset temperature of 76.5 K.

Investigations of the transport properties of 2H-TaS_2 flakes of different thicknesses have recently been reported to show an enhancement of the superconducting critical temperature up to 2.2K in the thinnest (~3.5 nm) samples studied.[3] Here we demonstrate that significant enhancements of the critical temperature can also be induced in thicker 2H-TaS_2 flakes using a DEME-TFSI ionic liquid top gate (Fig. 1). T_c is found to be enhanced still further upon application of a back gate voltage. The role of the electronic density of states and charge density waves on superconductivity in this material will be discussed.

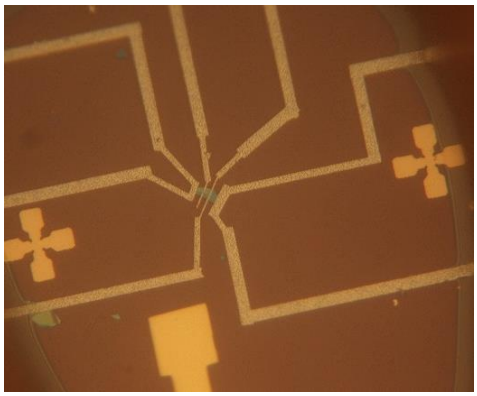

Figure 1: Optical image of a 2H-TaS2 FET device.

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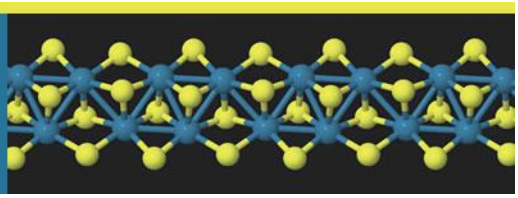

P.5 Controlled formation of an isolated miniband in bilayer graphene on an almost commensurate $\sqrt{3} \times \sqrt{3}$ substrate

D J Leech and M Mucha-Kruczyński

University of Bath, UK

We investigate theoretically the interplay between the effects of perpendicular electric field and incommensurability at the interface on the electronic properties of a van der Waals heterostructure [1] of bilayer graphene (BLG) and a semiconducting hexagonal substrate with a unit cell almost three times larger than that of graphene (e.g. In_2Te_2, InSe). The former introduces an asymmetry in the distribution of the electronic wave function between the layers and opens a band gap in the electronic spectrum, the size of which depends on the strength of the applied field [2]. The latter generates a long wavelength periodic moiré perturbation of graphene electrons which couples states in inequivalent graphene Brillouin zone corners and leads to the formation of minibands [3].

Using the form of the perturbation developed for the monolayer graphene system [3], we show that, depending on the details of the moiré perturbation, the miniband structure can be tuned from that with a single band gap at the neutrality point and overlapping minibands on the conduction/valence band side to a situation where a single narrow miniband is separated by gaps from the rest of the spectrum.

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P.6 Linear-Scaling DFT investigations of defect formation energies within TMDC lateral heterostructures

N Yeung and N Hine

University of Warwick, UK

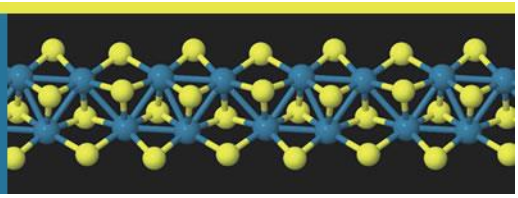
A lateral heterostructure is formed when two layered materials, such as transition metal dichalcogenides, are joined horizontally. Their properties are not nearly as well-known as the properties of individual monolayers or even vertical heterostructures. For example, there have been reports of enhanced photoluminescence in lattice-mismatched lateral heterostructures, but an atomistic understanding of such phenomena is not yet available. We have employed high-accuracy linear-scaling density functional theory calculations, using the ONETEP code, to provide theoretical predictions of the properties of WS_2–MoS_2 lateral heterostructures. The dependence of formation energies of vacancies on distance to the interface is examined, to examine the tendency of defects to segregate to the different regions.

P.7 Growth and characterisation of $TiSe_2$: A chiral charge density wave material

C Sayers and E Da Como

University of Bath, UK

Titanium diselenide ($TiSe_2$) is an intriguing member of the transition metal dichalcogenides (TMDs) which has semimetal character and peculiar charge ordering. Bulk 1T-$TiSe_2$ exhibits a (2 × 2 × 2) charge density wave (CDW) transition at 200 K which is enhanced in the monolayer[1], but the mechanism of its origin is still not fully



understood. Recently, the first evidence of a chiral CDW was found in 1T-$TiSe_2$ by STM and time-resolved optical polarimetry[2]. These chiral CDWs have been shown to exist in many ordered domains within a single sample. The dynamics of this ordering can be studied by the optical melting and recovery of CDW domains in $TiSe_2$. This leads to the possibility of selectively probing and controlling CDWs in 2D materials.

We have grown large single crystals of 1T-$TiSe_2$ from the elements by iodine vapour transport, and their quality has been confirmed by Raman spectroscopy. We present preliminary results of time-resolved optical experiments, such as femtosecond pump-probe spectroscopy and trARPES.

P.8 High photoresponsivity in graphene-multilayer WS_2 heterostructures with an ionic polymer gating

S Unal, J Mehew, E Torres Alonso, M Craciun and S Russo

University of Exeter, UK

Achieving high photoresponsivity, efficient photogeneration and fast response times in two-dimensional materials are important for creating the next generation of atomically thin photodetectors such as graphene and tungsten disulfide (WS_2). Although, graphene with its high carrier mobility and transparency makes it an excellent candidate for heterostructure materials. However the absence of a band gap and low light absorption in the visible range of optical spectrum limits its applications in optoelectronic devices. WS_2 is one of the transition metal dichalcogenides (TMDCs), as a semiconductor has a band gap of 2.1 eV which can be used in visible spectral range photodetectors. Hybrid structures can be used to overcome the limitations in graphene as well as providing high charge carrier transport.

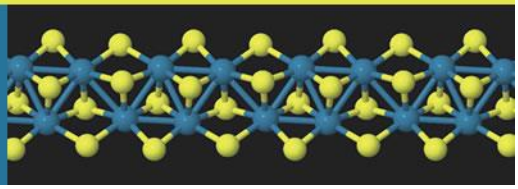
WS_2/Graphene heterostructure devices were fabricated with a transparent polymer top gate which enables gate transport measurements. Multilayer WS_2 is used to maximize absorption of the light and graphene with its high mobility which increases photoactivated charge carrier transport from the WS_2 to be collected by the Au electrodes. They were characterised electrically and optically. 473 nm laser is rastered to photocurrent map the device in order to identify the active area. The photocurrent is generated in the heterojunction between WS_2 and graphene. Furthermore, the heterostructure is bulk illuminated with a xenon lamp, and a monochromator provides modulation of the light frequency. Photoresponsivity with respect to wavelength is measured. This corresponds to the absorption of the WS_2. The spectral photoresponsivity can reach up to 650 nm observing A, B and C excitonic interactions along with absorption due to the direct band gap. The responsivity of 10^6 A/W is achieved, and the response time is on the milliseconds timescale. Hybrid structures of WS_2/graphene can be used in video imaging and future photodetector applications.

P.9 Computational study of the effect of single point defects on the electrical properties of MoS_2 bilayer

A Stroud[1], C Muratore[2], R Berry[3] and P A Derosa[1,4]

[1]Louisiana Tech University, USA, [2]University of Dayton, USA, [3]Air Force Research Lab, USA [4]Grambling State University, USA

Over the past decade, two dimensional materials like graphene have shown both unique electronic and mechanical properties making them attractive for applications in micro and nanoscale electronics. Transition metal dichalcogenides (TMDs), however, have been considered alternative materials for transistor and sensing applications. They show rather unique electronic properties, including a direct band gap, that changes with the number of layers, and becomes indirect when reduced to a monolayer. Here Density Functional Theory (DFT) in combination with Non-Equilibrium Green's Function (NEGF), as implemented in the Atomistix Toolkit (ATK) software



package, is used to study conductive and electronic properties in a MoS_2 twoprobe device model. The impact of single point defects on the electronic and conductive properties of the bilayers is studied. Information gathered from the device setup includes the density of states (DOS), transmission spectra, IV curves, transport pathways, and electron density.

P.10 Low wavenumber Raman determination of layer number in ReS_2 flakes

T Batten[1], L Hart[2] and D Wolverson[2]

[1]Renishaw plc, UK, [2]University of Bath, UK

In this work mechanically exfoliated flakes of ReS_2 with different thickness were characterised using Raman spectroscopy. The use of ultra-low frequency Raman filters (Eclipse filters) allowed the low wavenumber layer breathing modes and layer shear modes to be measured. The low wavenumber modes occur due to vibrations between layers of ReS_2, the frequency of these modes changes with increasing layer number, enabling straight forward determination of layer numbers up to 10 layers. In addition, when there is only a single layer of material no modes occur at all, making this a very quick and easy method for locating single layer flakes.

Raman spectroscopy is a non-contact, non-destructive tool that provides sub-micrometre information on the vibrational, crystal and electronic structure of materials. Raman spectroscopy is the ideal tool for investigating 2D materials as it can be used to determine layer number, stress/strain and electronic properties of these materials. Recent advances in instrumentation at Renishaw have made characterisation of these materials easier and more comprehensive, adding features such as ultrafast mapping (<1000 spectra/s), low wavenumber filters and automatic sample focus tracking capabilities.

A Raman maps was conducted over an area containing a number of Res_2 flakes of differing thicknesses. Analysis of low wavenumber bands and comparison to literature results [1], enabled the thickness of these flakes to be determined (Figure 1).

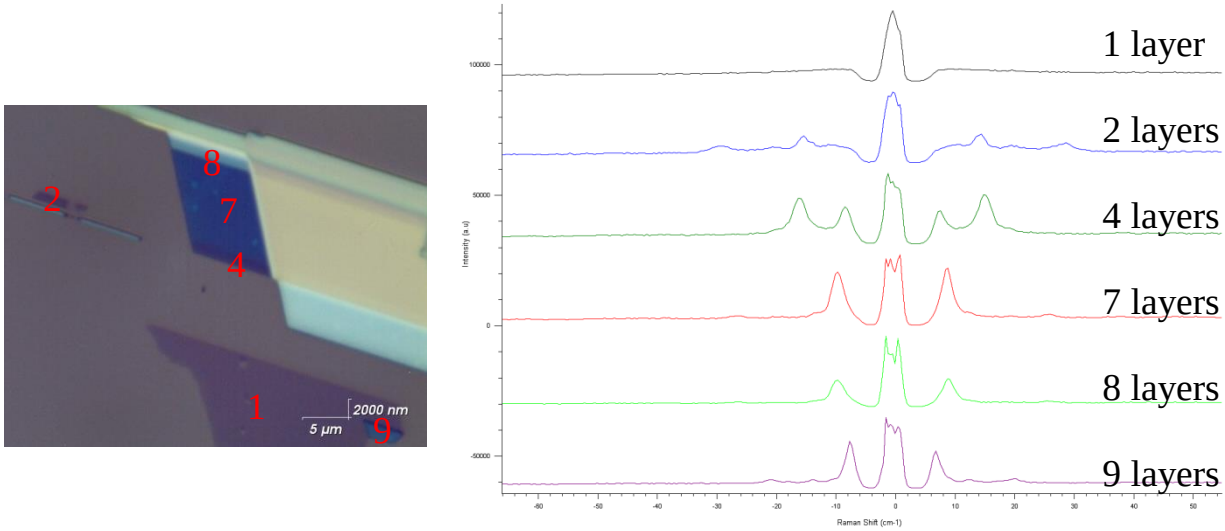


Figure 1 Optical image of flakes of different thicknesses and correspond low wavenumber Raman spectra

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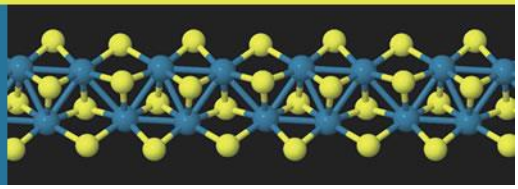

P.11 Rhenium disulphide and rhenium diselenide: lattice dynamics in anisotropic layered semiconductors

L Hart, S Hoye and D Wolverson

University of Bath, UK

Rhenium disulphide and rhenium diselenide are two of the less familiar members of the family of forty or so layered transition metal dichalcolgenides (TMDs) reviewed in the seminal work of Wilson and Yoffe (1969)[1]. Since the isolation of graphene and the current intense interest in monolayer semiconductors generally, the TMD family has attracted renewed attention and is proving to offer rich possibilities both for basic physics and for device applications. The TMD family contains metals, superconductors, and direct and indirect bandgap semiconductors and these can in principle be combined layer by layer to build up new device concepts[2].

The compounds $ReSe_2$ and ReS_2 are conventional semiconductors but are unusual members of the TMD family in that they (i) have a particularly low strength of interaction between layers – lower even than more familiar van der Waals materials such as MoS_2[3] – and (ii) they do not possess the most common hexagonal structure, but are triclinic with a relatively large number of atoms per unit cell. We show that in consequence their Raman spectra demonstrate a large number of zone-centre Raman active lattice modes which give one the ability to determine the orientation of the non-equivalent in-plane crystallographic axes in a few layer or monolayer sample[4]. In multi-layer devices, these materials will offer a controlled in-plane anisotropy and sensitivity to light polarization, for which Raman will be a useful diagnostic.

We present results of both experimental and first-principles computational studies of both materials in order to understand the observed Raman spectra and thus to highlight methods of measuring orientation suitable for use in a typical "Raman mapping" experiment. We establish some common features of the lattice dynamics of these two materials and we compare these also to the more exotic (and radioactive) technetium analogue, TcS_2, for which we have likewise calculated the zone-centre phonon spectrum and have predicted the Raman spectra.

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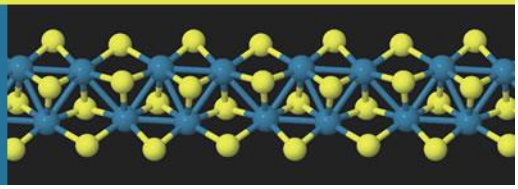
P.12 First-principles lattice dynamics of monolayer MoS_2

D Wolverson

University of Bath, UK

In order to realize the potential of single-layer or few-layer MoS_2 for novel nano-electronic devices, it is important to understand and to be able to measure the effects of strain when MoS2 is incorporated into device heterostructures. One suitable tool is Raman spectroscopy, whose usefulness for the investigation of strains in semiconductors with micrometre-scale spatial resolution is very well-established [1].

With this in mind, first-principles plane-wave pseudopotential calculations based on density functional perturbation theory(DFPT) [2] were used to determine the Grüneisen parameters for the E_{1g}, E_{2g}, A_{1g}, and A_{2u} phonon modes and



thus to predict the sensitivity of the Raman bands of monolayer MoS_2 to isotropic and shear strains. Given a knowledge of these basic parameters, the response of single-layer MoS_2 to more complicated strain situations can be modelled. The present simulations yielded values for other basic parameters (lattice parameter and in-plane stiffness) that were in good agreement with previous calculations and experimental values.

The calculations have been compared to experimental data, obtained in Manchester [3], on the strain-induced shifts of the Raman-active modes of monolayer and few-layer MoS2. Uniaxial strain was applied to thin-layer MoS_2 sandwiched between two layers of optically transparent polymer; the resulting shifts of the E_{2g} (~385.3 cm^{-1}) and A_{1g} (~402.4 cm^{-1}) Raman modes were found to be small but observable and were as predicted by DFPT on the basis of the external strain applied to the polymer. The interface between the polymer and the MoS_2 was found to remain intact through several strain cycles [3].

[1] D. Wolverson, in: C. Lamberti (Ed.), Characterization of Semiconductor Heterostructures and Nanostructures, Elsevier, Amsterdam, 2013.
[2] S. Baroni, S. de Gironcoli, A. Dal Corso, P. Giannozzi, Reviews of Modern Physics 73 (2001) 515-562.
[3] C. Rice, R.J. Young, R. Zan, U. Bangert, D. Wolverson, T. Georgiou, R. Jalil, K.S. Novoselov, Physical Review B 87 (2013) 081307.

P.13 nanoARPES of 2-dimensional TMD heterostructures

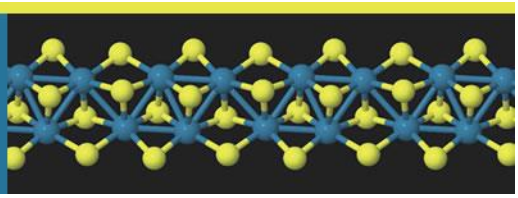
N C Teutsch[1], P V Nguyen[2], N Wilson[2], M Hoesch[3], P Dudin[3], N D M Hine[1], G C Constantinescu[4], X Xu[2], D H Cobden[2] and N R Wilson[1]

[1]University of Warwick, UK, [2]University of Washington, USA, [3]Diamond Light Source, UK, [4]University of Cambridge, UK

Layered heterostructures of 2-dimensional materials are attracting increasing attention due to their intriguing electronic and optical properties. A wide family of 2D materials, including transition metal dichalcogenides (TMDs), have now been identified and isolated in monolayer form, including semi-metals, semiconductors and insulators.

A pivotal aspect in understanding these monolayers is accurate determination of their electronic band structure and direct comparison with theory. With this focus, a key experimental technique which has been successfully utilized for characterisation is angle resolved photoemissions spectroscopy (ARPES). Conventional ARPES, which even for the leading synchrotron ARPES facilities has a beam size of at least 50 μm, enables direct band mapping of bulk crystals and epitaxially grown monolayers on single crystal substrates. However, mechanical exfoliation is typically used to isolate the 2D materials; producing flakes with micrometre scale lateral dimensions. Through successive transfers of these exfoliated materials, heterostructure stacks can be built, layer-by-layer, with precise alignment. The resultant heterostructures are typically only a few micrometres across, insufficient for conventional ARPES.

Here we show that recent advances in spatially resolved ARPES with sub micrometre resolution (nanoAPRES) can be used to address such heterostructures. Directly measuring angle resolved electronic structure from exfoliated flakes with high spatial and energy resolution and enabling direct determination of band parameters such as effective mass and spin orbit coupling induced band splitting, as well as band offsets and hybridisation induced band shifts. We apply this to several prototypical 2D material heterostructures, showing the change in electronic structure from monolayer to bulk WS_2, electronic structure of graphene on hBN, band alignments between graphene and TMD, and hybridisation induced shifts in a heterobilayer of $MoS_2/MoSe_2$. These results give new insight into band offsets and hybridisation effects in stacked 2D material heterostructures, and open up diverse possibilities for direct band mapping on 2D material devices.



P.14 AACVD Routes to tungsten disulfide on graphene

D Wolverson, J R Thompson, A J Rushworth and A L Johnson

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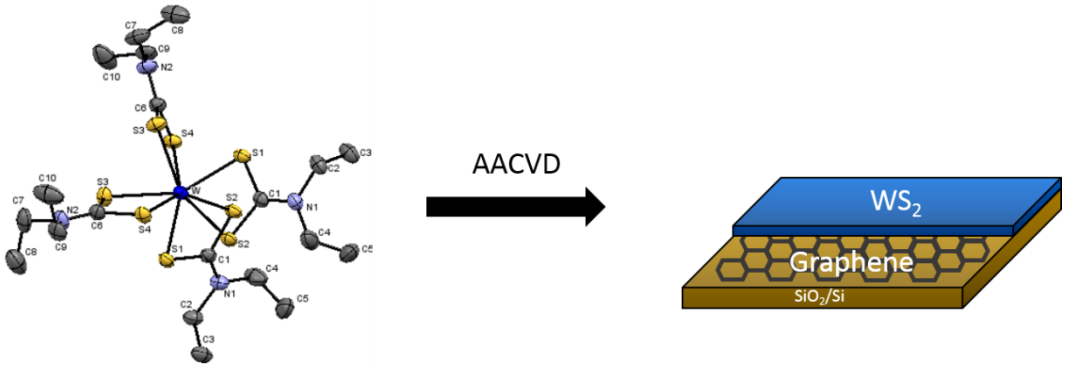
The discovery of two dimensional materials, principally graphene and transition metal dichalcogenides (TMDs), has opened up an exciting field of research into their production, properties and applications. The combination of these materials into layered heterostructures provides an opportunity to access improved properties and device functionality.[1] A major barrier to the introduction of these devices is the ability to deposit thin films of highly orientated TMDs using methodologies consistent with upscaling.

Mono- to 'few'-layer thin films of tungsten disulfide exhibit a direct band gap, as well as a high absorption coefficient, making it a strong candidate for use in photovoltaic, thermoelectric or FET devices.[2] Many of these applications require a transparent conducting layer for which graphene is the ideal choice. Herein, we report the deposition of tungsten disulfide thin films using aerosol assisted chemical vapor deposition (AACVD) with the single-source precursor, tetrakis(diethyldithiocarbamato)tungsten(IV). Direct deposition on graphene produced highly crystalline films less than 10 nm thick, as confirmed by Raman spectroscopy, PXRD, SEM, EDS and AFM. The resulting material is compared to monolayer tungsten disulfide films on graphene deposited from WO_3 and S.



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P.15 Inorganic graphene materials: Novel precursors for TiS_2, ZrS_2 and HfS_2 production

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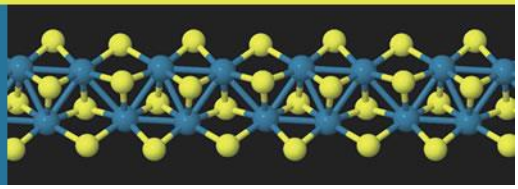
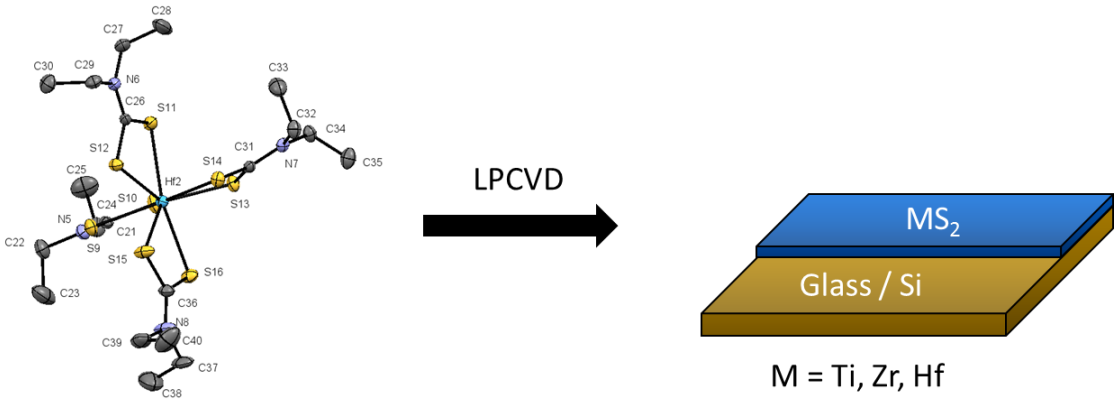
Transition metal dichalcogenides (TMDs) possess lamellar structures similar to that of graphene and exhibit wide ranging electrical properties. These materials are ideally suited to incorporation in thin, flexible electronic devices such as photovoltaics, thermoelectrics, field effect transistors and batteries. The major obstacle to the production of these devices is the ability to form large area, high quality thin films of these materials. Chemical vapour deposition (CVD) is already established as a technique for depositing large scale thin films of materials such as metal oxides but little has been developed for the deposition of TMDs.



While there is considerable literature on the deposition of group VI sulfides there is little work on the formation of group IV sulfide thin films. Titanium disulfide is a promising cathode material for Li-ion batteries and zirconium/hafnium disulfides exhibit advantageous semiconducting properties. We present the scalable deposition of titanium disulfide, zirconium disulfide and hafnium sulfide thin films using the precursor $M(S_2CNEt_2)4$ (M = Ti, Zr and Hf) under low pressure conditions (LPCVD). Films were analysed using Raman spectroscopy, PXRD, SEM, EDS and AFM.



P.16 Defects and dopants in WSe_2 and their local electronic characterization

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Defects and dopants in transition metal dichalcogenides (TMDs) are local atomic modifications through which electronic and magnetic properties of these materials can be controllably affected. Here we focus on WSe_2, which is one of the semiconductor transition metal dichalcogenides with strong potential in both spintronics and valleytronics. Using scanning tunnelling microscopy and spectroscopy (STM/STS) we image, characterize and assign atomic structure to a variety of atomic scale defects in WSe_2 crystals, as well as identify their signature electronic modification induced in the local density of states. Similar investigations are extended to metallic decorating dopants (individual atoms and few-atom nanocrystals).

P.17 Topological ladder in the metallic TMD 1T-$PdTe_2$

O J Clark[1], M S Bahramy[2,3], L Bawden[1], J M Riley[1,4], S P Cooil[5], V Sunko[1,6], M Jorge[5], J W Wells[5], M Leandersson[7], T Balasubramanian[7], T K Kim[4], M Hoesch[4], T Sasagawa[8], T Eknapakul[9], W Meevasana[9] and P D C King[1]

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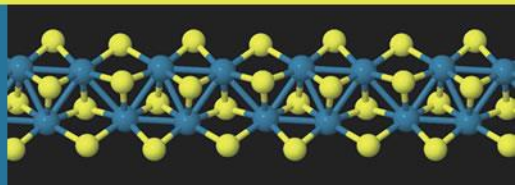
Recent work has established transition metal dichalcogenides (TMDs) as powerful compounds in which to probe the importance of spin-orbit coupling (SOC) derived effects in solids. The diversity in properties and potential applications offered by this class of materials is staggering, from orbital character coupled charge density wave



phases [1] to strong spin polarisations of their electronic states, exhibiting spin-valley locking in both non-centrosymmetric monolayer [2] and centrosymmetric bulk [3] systems. Here, we will show that TMDs can also be host to topological phenomena, revealing a rich array of SOC-induced topologically non-trivial states in 1T-$PdTe_2$. Combining direct electronic structure measurements from angle-resolved (as well as spin-resolved) photoemission spectroscopy (ARPES) with first-principles calculations, we will address the origins and nature of a bulk Dirac point and two topologically non-trivial surface states in this system, derived entirely from chalcogen p-bands. Through this, we shed new light on the nature of topological phase transitions in general, and how non-trivial band topology may be obtainable in multiple compounds across the TMD family.

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[3] J. Riley et al., Nature Phys. 10 (2014) 835

P.18 Spin-valley locking in the normal state of a transition-metal dichalocogenide superconductor

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2H-$NbSe_2$ is a metallic transition metal dichalcogenide, which hosts instabilities to a charge density wave phase at 33 K, and exhibits superconductivity at $\sim$ 7 K. [1] The origins and nature of these collective states have been fervently debated since their discovery four decades ago. To date, however, they have been assumed to emerge from a normal state of spin-degenerate quasiparticles. In contrast, from spin- and angle-resolved photoemission measurements, supported by first principles calculations, we reveal that the normal state Fermi surface hosts a complex spin texture. We uncover a rich spin-valley locking of the form also observed in the semiconducting materials of the same family,[2-5] and consistent with the recent observation of so-called Ising pairing in the superconducting state of monolayer $NbSe_2$.[5] We find that for the bulk compound there is persistent spin polarisation, which becomes intrinsically linked to the electronic dimensionality, showing a significant dependence on the out-of- plane momentum. This imposes restrictions on the form of the superconducting order parameter, prompting a reinterpretation of the mechanism for and properties of the collective phases in this and related materials.

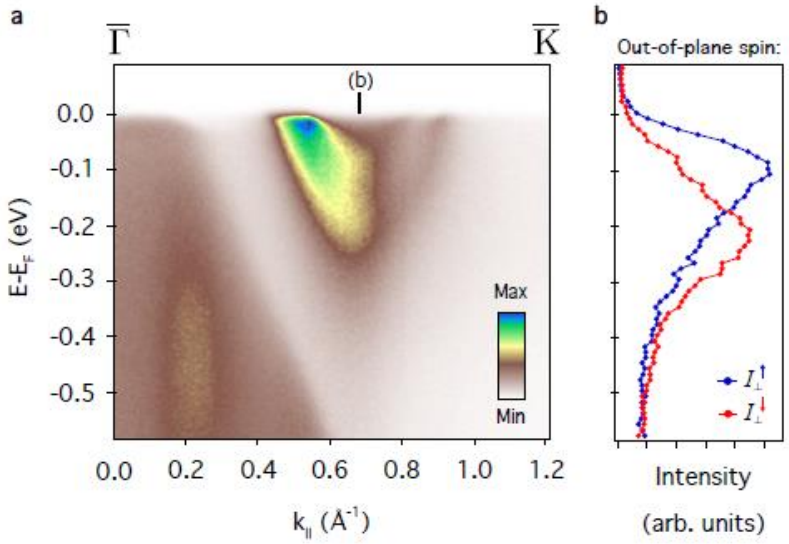

Figure 1: **Spin polarisation in $NbSe_2$** (a) Angle-resolved photoemission measurement along the Γ - K direction. (b) Spin resolved energy distribution curve showing strong out-of-plane spin polarisation of the bands crossing the Fermi level.

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[4] Riley, J. M. *et al.*, Nature Phys. **10** 11 (2014).
[5] Xi, X. *et al.*, Nature Phys. *Advanced Online Publication* (2015) DOI:10.1038/nphys3538

P.19 Dipolar exciton-polaritons in electric and magnetic fields

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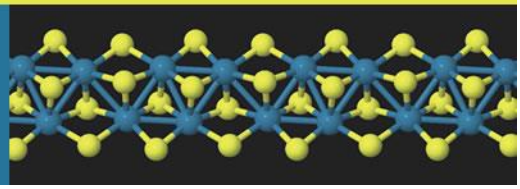
Exciton-polaritons in semiconductor quantum wells (QWs) have been studied intensively in recent years. This is due to the ability to observe quantum condensation in these systems, stimulated by the development of new quantum technologies [1]. We present a precise calculation of polariton states formed from the coupling of a spatially-indirect exciton in coupled quantum wells (CQWs) to the optical mode of a microcavity [2]. We include the presence of electric and magnetic fields applied perpendicular to the QW plane. A highlight of our approach is that it is transferable to other 2D systems such as various transition metal dichalcogenide monolayers and bilayers. These materials are intriguing to study because of the large exciton binding energy that permits polariton effects to persist to high temperatures.

To study the electric and magnetic field dependence of exciton states, we solve the exciton Schrödinger equation in real space in 3D [3-5] and calculate the absorption spectrum. For the ground state exciton, we study the dipole moment, oscillator strength, binding energy and magnetic field induced effective mass enhancement. Using the scattering matrix method, we solve Maxwell's equation for light inside a microcavity with embedded CQWs using a non-local susceptibility to describe the exciton polarization.



We calculate the field dependence of the reflectivity spectrum for the InGaAs microcavity-embedded CQWs that were studied in [2] (see Fig. 1a). Our model predicts the existence of polaritons which are in the strong coupling regime and at the same time possess a large static dipole moment (Figs. 1e-g). In particular, we demonstrate that a magnetic field can compensate for the reduction in polariton brightness (Figs. 1b-d) that occurs when an electric field impresses a dipole moment on the polariton. This is made explicit in Figs. 1d and 1g where the electric field is chosen to compensate for the diamagnetic shift. A substantial increase in dipole moment is achieved at the cost of a small decrease in brightness. Applying both fields therefore provides a means to maximise the polariton-polariton interaction which is useful for studying and harnessing many body effects.

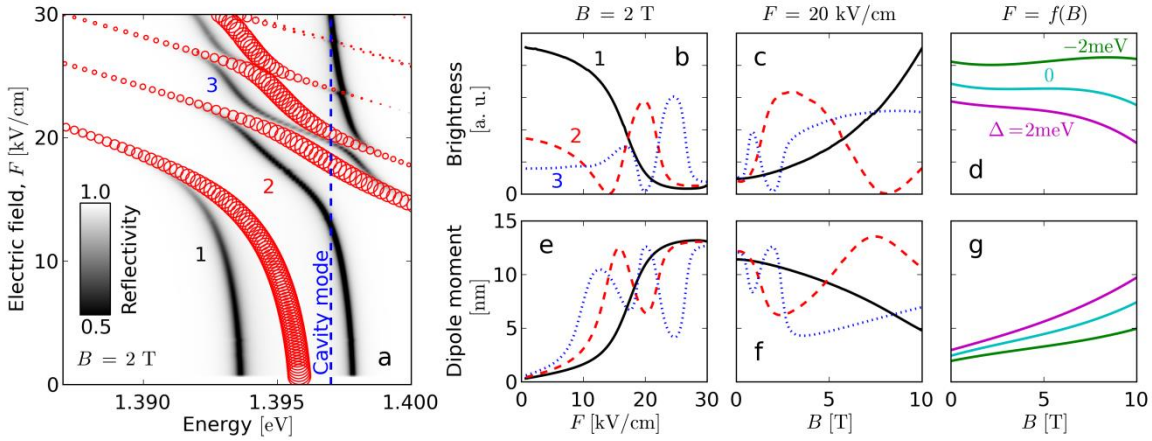


Fig.1: (a) Electric field dependence of the magneto-polariton reflectivity spectrum (greyscale). Exciton states are shown by circles with area proportional to oscillator strength. Brightness (b,c) and dipole moment (e,f) of the lowest three polariton states as a function of electric field (b,e) and magnetic field (c,f). Brightness (d) and dipole moment (g) of the polariton ground state with electric field, F = *f(B)* chosen to keep a fixed detuning Δ between the exciton ground state and the cavity mode.

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