Flatlands beyond Graphene 2016

Bled, Slovenia, July 5–8

book of abstracts

Welcome to Flatlands beyond Graphene 2016!

The Flatlands beyond Graphene conference series, initiated in Bremen, Germany (2013), and subsequently held in Dublin, Ireland (2014), and in Ramat Gan, Israel (2015), aims to promote discussions and information exchange across the frontiers of research in the field of two-dimensional materials. International scientists with common professional interests in the growth, processing, chemistry, structure, electronics, photonics, and fundamental physics of two-dimensional materials will gather on the sunny side of the Alps in a friendly and informal atmosphere to share their experimental and theoretical expertise. For up-to-date practical information about this conference please refer to http://flatlands2016.ijs.si/.

We wish you a stimulating conference and a pleasant stay in Bled!

The organizers:
Christoph Gadermaier (conference chair)
Sabina Padežnik (conference secretary)
Tetiana Borzda
Matej Prijatelj
Jure Strle
Victor Vega-Mayoral
Daniele Vella

Scientific advisory board:
Maya Bar Sadan (Ben Gurion University, Beer Sheva, Israel)
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Flatlands beyond Graphene 2016 has been organized in the framework of the Marie-Curie ITN project "MoWSeS".

Exhibitors:

cover photo: Milan Janša

TUESDAY 5th JULY 2016

8:00–8:45	**Registration**	
8:45–9:00	**FLATLANDS 2016 OPENING CEREMONY**	
	CHAIR: Reshef Tenne	
9:00–9:35	**Andras Kis** (EPFL, Switzerland) 2D dichalcogenide electronic materials and devices	◑
9:35–9:55	**Maja Remškar** (Jožef Stefan Institute, Slovenia) Quasi-two-dimensional Mo-S-I crystals	◔
9:55–10:30	**Janice L. Musfeldt** (University of Tennessee, USA) High pressure vibrational properties of WS_2 nanotubes	◑
	COFFEE BREAK	
	CHAIR: Janice L. Musfeldt	
10:55–11:30	**Paulina Plochocka** (Laboratoire National des Champs Magnétiques Intenses, France) Magneto excitons in atomically thin TMDs	◑
11:30–11:50	**Maya Bar Sadan** (Ben Gurion University, Israel) Designing doped transition metal dichalcogenides as improved photocatalysts	◔
11:50–12:25	**Zheng Liu** (Nanyang University, Singapore) Development of novel transitional metal dichalcogenides using chemical vapour deposition	◑
12:25–12:45	**Lena Yadgarov** (Tel Aviv University, Israel) Near-field imaging of exciton-plasmon wave functions confined in WS_2 nanotube	◔
	LUNCH	
	CHAIR: Maja Remškar	
14:15–14:50	**Alan Seabaugh** (University of Notre Dame, USA) Electric-double-layer field-effect transistors using polyethylene-oxide cesium perchlorate on two-dimensional materials	◑
14:50–15:10	**Yen-Cheng Kung** (EPFL, Switzerland) Flexible TFTs and circuits based on monolayer MoS_2	◔
15:10–15:45	**Claudia Backes** (University of Heidelberg, Germany, and Trinity College Dublin, Ireland) How to make monolayer-rich liquid-exfoliated 2D materials suitable for fundamental studies	◑
15:45–16:05	**Edward A. Lewis** (University of Manchester, United Kingdom) Top-down and bottom-up routes to solution processable nanosheets: size control, doping, and applications	◔
16:05–16:25	**Ravi S. Sundaram** (Oxford Instruments Plasma Technology, United Kingdom) CVD growth of 2-dimensional MoS_2 and heterostructures with graphene	◔
	COFFEE BREAK	
	CHAIR: Paulina Plochocka	
16:50–17:25	**Thomas Heine** (University of Leipzig, Germany) Noble metal transition metal dichalcogenides	◑
17:25–17:45	**Andrew Harvey** (Trinity College Dublin, Ireland) Determination of length from scattering spectra of liquid exfoliated layered double hydroxides and their use for electrochemical applications	◔
17:45–18:05	**Mathieu Massicotte** (ICFO, Spain) Photo-thermionic effect in graphene-based heterostructures	◔
18:05–18:25	**Jenya Tilchin** (Solid State Institute, Technion, Israel) Magneto-optical properties of individual perovskite nanocrystal	◔
18:30–21:00	**POSTER SESSION**	

WEDNESDAY 6th JULY 2016

CHAIR: Andras Kis		
8:45–9:30	**Reshef Tenne** (Weizmann Institute of Science, Israel) 2D materials: macroscopic and nanoscopic viewpoint	◕
9:30–9:50	**Nikos Papadopoulos** (TU Delft, The Netherlands) Boron nitride encapsulated MoS_2 photodetectors with 1T/1T'-MoS_2 electrodes	◔
9:50–10:10	**Conor P. Cullen** (Trinity College Dublin, Ireland) X-ray photoelectron spectroscopy study of the reversible functionalisation of MoS_2	◔
10:10–10:30	**Bojana Višić** (Weizmann Institute of Science, Israel) Optical properties of WS_2 nanotubes	◔
COFFEE BREAK		
CHAIR: Thomas Heine		
10:55–11:30	**Dongwon Yoo** (Yonsei University, South Korea) Effective chemical approach for single- to multi-layer two-dimensional transition metal chalcogenide nanosheets	◑
11:30–11:50	**Leonardo Medrano Sandonas** (TU Dresden) Quantum thermal transport in two-dimensional materials: a NEGF-DFTB study	◔
11:50–12:25	**Thomas Mueller** (Vienna University of Technology, Austria) Generation and detection of light in 2D materials and heterostructures	◑
12:25–12:45	**Nikodem Czechowski** (Institute of Physics, PAS, Poland) Enhancement of photoluminescence intensity of atomically flat, liquid exfoliated WS_2 monolayers utilizing plasmon excitation	◔
LUNCH		
CHAIR: Tobias Korn		
14:15–14:50	**Janina Maultzsch** (TU Berlin, Germany) Resonance Raman spectroscopy and excitons in few-layer 2D materials	◑
14:50–15:10	**Tsachi Livneh** (Departments of Physics, NRCN, Israel) High pressure and low temperature Raman scattering in inorganic fullerenes of MoS_2	◔
15:10–15:45	**Giulio Cerullo** (Politecnico di Milano, Italy) Ultrafast optical response of single-layer MoS_2	◑
15:45–16:05	**Marc Raupach** (Vrije University, The Netherlands) Developing a method to calculate response properties for two-dimensional materials in the BAND program	◔
16:30–19:30	**EXCURSION**	
19:30–22:00	**CONFERENCE DINNER**	

THURSDAY 7th JULY 2016

CHAIR: Maya Bar Sadan		
8:45–9:20	**Takayoshi Sasaki** (National Institute for Materials Science, Japan) Function design *via* organization of 2D oxide nanosheets at nano- to mesoscale	◑
9:20–9:40	**Egbert Zojer** (Graz University of Technology, Austria) Electrostatic design of the electronic properties of 2D materials	◔
9:40–10:15	**Niall McEvoy** (Trinity College Dublin, Ireland) Thermally assisted conversion – a versatile route for the synthesis of transition metal dichalcogenides	◑
10:15–10:35	**Elena del Corro** (Academy of Science of the Czech Republic) Uniaxial compression in monolayer MoS_2 and WS_2	◔
COFFEE BREAK		
CHAIR: Giulio Cerullo		
10:55–11:30	**Ronen Rapaport** (The Hebrew University of Jerusalem, Israel) Two-dimensional dipolar exciton fluids	◑
11:30–11:50	**Tetiana Borzda** (Jožef Stefan Institute, Slovenia) Mechanism of charge carrier generation in few-layer MoS_2	◔
11:50–12:25	**Goki Eda** (National University of Singapore, Singapore) Electro-optical properties of monolayer semiconductors	◑
12:25–12:45	**Victor Vega-Mayoral** (Jožef Stefan Institute, Slovenia) Relaxation processes of photogenerated charges in MoS_2 and WS_2	◔
LUNCH		
CHAIR: Claudia Backes		
14:15–14:50	**Tobias Korn** (University of Regensburg, Germany) Twist-induced tuning of interlayer coupling in monolayer dichalcogenide heterostructures	◑
14:50–15:10	**Daniele Vella** (Jožef Stefan Institute, Slovenia) Giant unconventional electroabsorption in monolayer MoS_2	◔
15:10–15:45	**Valeria Nicolosi** (Trinity College Dublin, Ireland) Processing and applications of liquid-phase exfoliated two-dimensional nanosheets	◑
15:45–16:05	**Nataša Vujičić** (Institute of Physics, Croatia) Optical properties of WS_2/MoS_2 heterostructures from chemical vapor deposition	◔
16:05–16:25	**Artem Mishchenko** (University of Manchester, United Kingdom) Tunnelling in van der Waals heterostructures	◔
COFFEE BREAK		
CHAIR: Egbert Zojer		
16:50–17:25	**Clotilde S. Cucinotta** (Trinity College Dublin, Ireland) A theoretical ride over 2D landscapes	◑
17:25–17:45	**Dmitry Ovchinnikov** (EPFL, Switzerland) Electrical transport properties of ReS_2 with polymer electrolyte gating in the high-doping limit	◔
17:45–18:05	**Agnieszka Kuc** (University of Leipzig, Germany) Electronic properties of 2D transition-metal chalcogenides beyond MoS_2	◔
18:05–18:25	**Jens Kunstmann** (TU Dresden, Germany) The importance of steric effects for interlayer interactions in 2D homo- and heterostructures	◔
18:25–18:45	**Juan F. Sánchez-Royo** (University of Valencia, Spain) Morphological manipulation of the luminescent response of atomically thin indium selenide nanosheets	◔

FRIDAY 8th JULY 2016

CHAIR: Niall McEvoy		
8:45–9:20	**Andor Kormányos** (University of Konstanz, Germany) Magnetoconductance oscillations and edge states in semiconducting monolayer transition metal dichalcogenides	◑
9:20–9:40	**Matej Prijatelj** (Jožef Stefan Institute, Slovenia) Ambient intercalation and rapid expansion of MoS_2 crystals	◔
9:40–10:15	**Andres Castellanos-Gomez** (IMDEA Nanoscience, Spain) Novel narrow gap 2D semiconductors for optoelectronics and straintronics	◑
10:15–10:35	**Dumitru Dumcenco** (EPFL, Switzerland) CVD growth of transition metal diselenides	◔
COFFEE BREAK		
CHAIR: Thomas Mueller		
10:55–11:30	**Dragan Mihailović** (Jožef Stefan Institute, Slovenia) Ultrafast memristive switching utilising hidden collectively ordered many-body quantum states in 1T-TaS_2	◑
11:30–11:50	**Deniz Çakir** (University of Antwerp, Belgium) Peculiar piezoelectric properties of two-dimensional materials	◔
11:50–12:25	**Simin Feng** (University Park, USA) Tuning the properties of two-dimensional materials by doping and heterostacking	◑
12:25–12:45	**Kanudha Sharda** (Imperial College London, United Kingdom) Electrochemical nature of ionic liquid gated Bi_2Te_3 transistors	◔
LUNCH		
CHAIR: Nataša Vujičić		
14:15–14:35	**Toby Hallam** (Trinity College Dublin, Ireland) Multilayer TMDC synthesis and phase conversion	◔
14:35–14:55	**Alessandro Surrente** (Laboratoire National des Champs Magnétiques Intenses, France) Static and dynamic optical properties of monolayer black phosphorus	◔
14:55–15:15	**Meinrad Sidler** (ETH Zürich, Switzerland) Fermi polaron-polaritons in $MoSe_2$	◔
15:15–15:35	**Vivek Pachauri** (University of Applied Sciences Kaiserslautern, Germany) Label-free optical biosensor platform based on 2D inorganic semiconductors	◔
15:35–15:55	**Abdou Hassanien** (Jožef Stefan Institute, Slovenia) Frustration and order in insulating and superconducting monolayers of $(BETS)_2GaCl_4$ on Ag(111)	◔
15:55–16:05	**CLOSING REMARKS**	

2D dichalcogenide electronic materials and devices

Andras Kis

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The discovery of graphene marked the start of research in 2D electronic materials which was expanded in new directions with MoS_2 and other layered semiconducting materials. They have a wide range of promising potential applications, including those in digital electronics, optoelectronics and flexible devices. Combining 2D materials in heterostructures can increase their reach even further.

In my talk I will review the status of our research in 2D transition metal dichalcogenides (TMDCs) and present our current level of understanding on the influence of contacts, material quality and the environmental effects on 2D materials, all critical for achieving high performance levels in devices based on 2D semiconductors. I will also update on our efforts to achieve high operation frequencies in scaled TMDC devices. Next, I will show our work on atomically thin rhenium disulphide (ReS_2) liquid-electrolyte gated transistors with atypical behaviour at high charge densities related to the peculiar band structure of this material. Finally, I will present our recent work on electromechanical response of MoS_2 and graphene.

Quasi-two-dimensional Mo-S-I crystals

Maja Remškar[a], Ana Varlec[a,b], Janez Jelenc[a], Srečko D. Škapin[a], Sara Fathipour[c], Alan Seabaugh[c], and Zvonko Jagličič[d]

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[b]*A. P. E. Research, Area Science Park, Basovizza Campus, Building Q, Trieste, Italy*
[c]*University of Notre Dame, Department of Electrical Engineering, Notre Dame, Indiana, USA*
[d]*Institute for Physics, Mathematics and Mechanics, Ljubljana, Slovenia*
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Superconductive compound $Mo_6S_6I_2$ belongs to cluster compounds composed of Mo_6X_8 units (X = S, Se, Te), where part of chalcogen atoms are replaced by iodine as monovalent substituents[1]. In contrary with many other so-called Chevrel phases with the general formula $Mo_6S_{8-x}I_x$, which are of needle-like morphology and differ in the site occupation by sulphur and iodine, like $Mo_6S_2I_8$[2] and $Mo_6S_4I_6$[3], the $Mo_6S_6I_2$ compound shows a low degree of morphological anisotropy and crystallizes in three-dimensional semi-cubic shape[4]. Its structure is described as the hexagonal rhombohedral structure of the $PbMo_6S_8$ type with the lattice parameters: a_R = 6.563 Å and α_R = 94.5 Å. The critical temperature (T_c) for the superconducting transition in $Mo_6S_6I_2$ is 14 K.

We report on the first quasi-2-dimensional Mo-S-I compound, which grows epitaxially on the surface of $Mo_6S_6I_2$ crystals in shape of thin and rigid belts. Crystal structure of the belts is similar to $Mo_6S_2I_8$, but not the same. Results of structural characterization of this new Mo-S-I compound in comparison with the $Mo_6S_6I_2$ cubes and $Mo_6S_2I_8$ nanowires will be presented and growth mechanism will be discussed. High resolution images and results of vibrational and electric analysis will be shown.

[1] A. Perrin, C. Perrin, and M. Sergent, "Octahedral clusters in molybdenum(II) and rhenium(III) chalcohalide chemistry", *J. Less-Common Met.* **137** (1988) 241.

[2] C. Perrin, M. Sergent, "A new family of monodimensional compounds with octa-hedral molybdenum clusters. $Mo_6X_8Y_2$ (X = halogen, Y = chalcogen)", *J. Chem. Res. (S)* **2** (1983) 38.

[3] M. Remskar, A. Mrzel, M. Virsek, M. Godec, M., Krause, A. Kolitsch, A. Singh, A. Seabaugh, "The MoS_2 Nanotubes with Defect-Controlled Electric Properties", *Nanoscale Res Lett* **6**:26 (2011).

[4] M. Sergent, Ø. Fisher, M. Decroux, C. Perrin, R. Chevrel, "Stabilization of Mo_6S_8 by halogens; new superconducting compounds: $Mo_6S_6Br_2$, $Mo_6S_6I_2$, *J. of Solid State Chem*. **22** (1977) 87.

High pressure vibrational properties of WS_2 nanotubes

J. L. Musfeldt[a], K. R. O'Neal[a], T. Auther[a], J. G. Cherian[a], A. Zak[b], R. Tenne[c], and Z. Liu[d]

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We bring together synchrotron-based infrared and Raman spectroscopies, diamond anvil cell techniques, and an analysis of frequency shifts and lattice dynamics to unveil the vibrational properties of multiwall WS_2 nanotubes under compression[1]. While most of the vibrational modes display similar hardening trends, the Raman-active A_{1g} breathing mode is almost twice as responsive, suggesting that the nanotube breakdown pathway under strain proceeds through this displacement (Fig. 1). At the same time, the previously unexplored high pressure infrared response provides unexpected insight into the electronic properties of the multiwall WS_2 tubes. The development of the localized absorption is fit to a percolation model, indicating that the nanotubes display a modest macroscopic conductivity due to hopping from tube to tube.

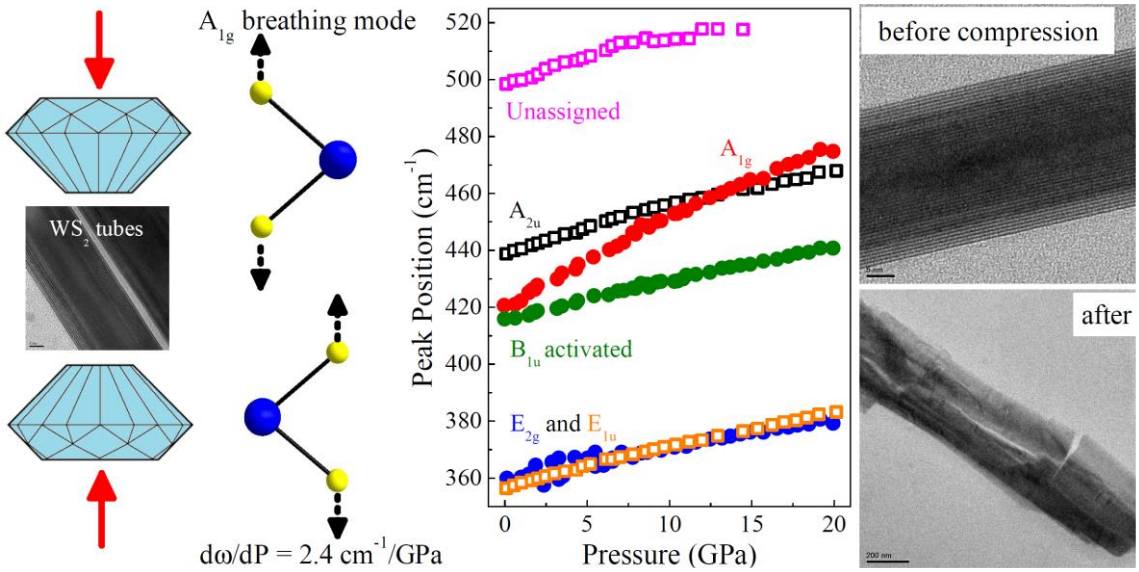

Figure 1 Schematic images of the diamond anvil cell, the displacement pattern for the A_{1g} breathing mode, a comparison of infrared and Raman mode trends with pressure, and TEM images of the tubes before and after compression.

[1] K. R. O'Neal, J. G. Cherian, A. Zak, R. Tenne, Z. Liu, and J. L. Musfeldt, "High pressure vibrational properties of WS_2 nanotubes", *Nano Lett.* **16**, 993–999 (2016).

Magneto excitons in atomically thin TMDs

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In this talk I will discuss the optical and magneto-optical properties of excitons in transition metal dichalcogenides (TMDs). I will show that optical spectroscopy in high magnetic fields reveals the very different nature of carriers in monolayer and bulk transition metal dichalcogenides. In monolayer WSe_2 obtained by mechanical exfoliation, the exciton emission shifts linearly with the magnetic field and exhibits a splitting, which originates from the magnetic field-induced valley splitting. The monolayer data can be described using a single particle picture with a Dirac-like Hamiltonian for massive Dirac fermions, with an additional term to phenomenologically include the valley splitting. In contrast, in bulk WSe_2, where the inversion symmetry is restored, transmission measurements show a distinctly excitonic behavior with absorption to the 1s and 2s states. Magnetic field induces a spin splitting together with a small diamagnetic shift and cyclotron-like behavior at high fields, which is best described within the hydrogen model[1]. In the latter part of the talk I will switch to the optical properties of large area CVD grown MoS_2 and $MoSe_2$. The samples were of the size of hundreds of square microns[2]. Comparison between μPL and μ-transmission spectra allows us to identify emission/absorption from the A and B excitons originating from spin-orbit split levels in the valence and conduction bands, together with emission/absorption from bound excitons at low temperatures. The measured life time of the neutral exciton is comparable to the lifetime measured in small flakes obtained by mechanical exfoliation. Using magneto-transmission spectroscopy we have investigated the valley Zeeman splitting. The extracted values of the valley *g*-factors for both A- and B-exciton are similar with $g_v \approx 4.5$. The samples are expected to be strained due to the CVD growth on sapphire at high temperature (700 °C). However, the estimated strain, which is maximum at low temperature, is only 0.2%. Theoretical considerations suggest that the strain is too small to significantly influence the electronic properties. This is confirmed by the measured value of valley *g*-factor, and the measured temperature dependence of the band gap, which is almost identical for CVD and mechanically exfoliated MoS_2. Our results show that the deviations from valley factor $g_v = 4$ do not originate from strain. Finally, we have observed very strong, magnetic field induced, polarization for $MoSe_2$. It is an intriguing effect as a zero magnetic field valley polarization is observed for all TMDs with the exception $MoSe_2$[3].

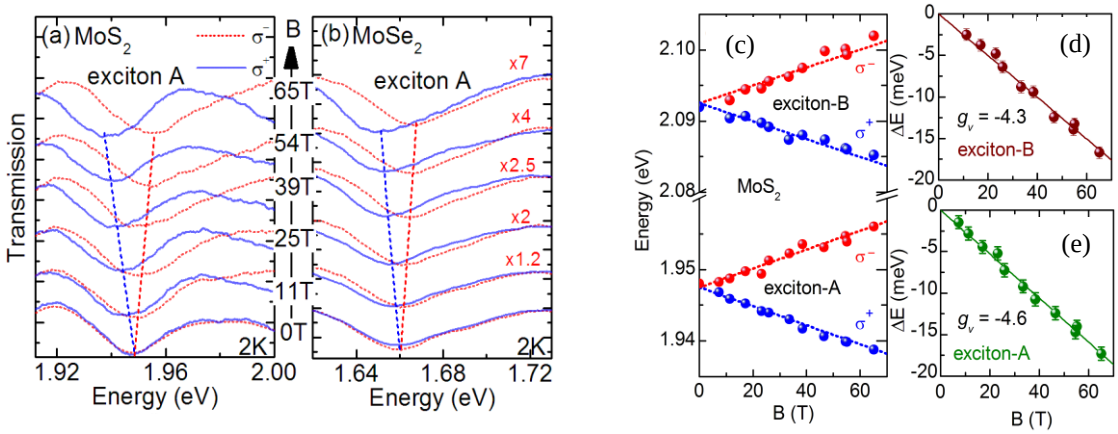

Figure 1 (a–b) Typical low temperature magneto-transmission spectra for MoS_2 and $MoSe_2$. (c) Transition energies for the A- and B-excitons in monolayer MoS_2. (d–e) The A- and B-exciton valley splitting.

[1] A. Mitioglu *et al.*, *Nano Letters* **15**, 4387 (2015).
[2] D. Dumcenco *et al.*, *ACS Nano* **9**, 4611 (2015).
[3] A. Mitioglu *et al.*, submitted.

Designing doped transition metal dichalcogenides as improved photocatalysts

Maya Bar Sadan

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E-mail: barsadan@bgu.ac.il

Currently, Pt is the primary catalyst for hydrogen production, but it is scarce and expensive and therefore efforts are focused on finding alternatives. Promising candidates are nanostructured MoS_2 and other transition metal di-chalcogenides (TMD). Here I present the rational design of a new class of sophisticated tailor-made nanoflower photocatalysts, produced for specific requirements, with a scalable reaction mechanism, durability and low cost. TMD nanoflowers are unique structures, since their morphology provides multiple catalytic sites and allows tuning the light absorbing properties to the solar radiation. The nanoflowers offer improved conductivity, charge separation capabilities and light absorbing properties, and in addition the enrichment of specific populations of catalytic sites by doping. Rational design of TMD photocatalysts is important not only for hydrogen evolution, but also for several other photocatalytic processes, where specific catalytic sites are designed on a robust, light absorbing skeleton.

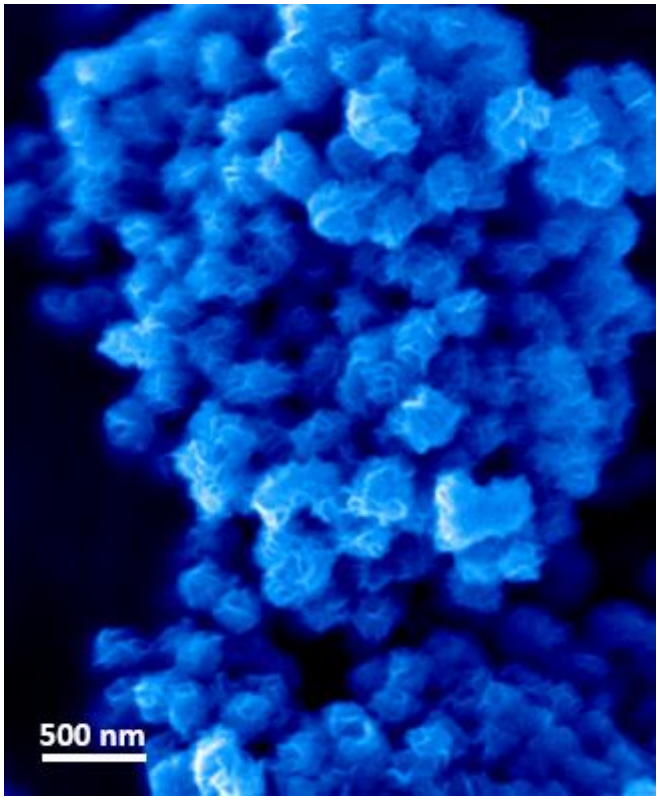

Figure 1 SEM image of $MoSe_2$ nano-flowers.

Development of novel transitional metal dichalcogenides using chemical vapour deposition

Zheng Liu

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The one-atom-thick layers like graphene have attracted tremendous interests in these years, which open a window to the landscape of the two-dimensional (2D) materials. Using chemical solid reaction and chemical vapour deposition, we have successfully synthesized a wide spectrum of transitional metal dichalcogenides materials including:

1. Binary 2D materials: MoS_2, WSe_2, $MoSe_2$, WSe_2, $MoTe_2$, WSe_2, ReS_2, $ReSe_2$, PtS_2, $PtSe_2$, PdS_2, $PdSe_2$, $NbSe_2$, SnS_2, SnSe, $SnSe_2$, TiS_3, $HfSe_3$, $HfTe_3$, $TiSe_2$, $TaTe_2$, $TaSe_2$, etc.

2. Ternary and multi-component 2D materials: $Mo_xW_{1-x}S_2$, $MoWTe_4$, $MoS_{2x}Se_{2(1-x)}$, $WSe_{2x}Te_{2(1-x)}$, $ReS_{2x}Se_{2(1-x)}$, etc.

3. Heterostructured 2D materials: MoS_2/WS_2, $WSe_2/MoSe_2$, etc.

4. Organic/Inorganic heterostructures: MoS_2/Rubrene, etc.

Potential applications of TMDs have been developed, such as ultrasound, high-temperature oxidation-resistant coatings, 2D anisotropic electronics (FETs, resonators and photodetectors), energy harvester, lithium ion battery and catalyst and wearable devices etc. These applications pave a promising way to the large scale applications of 2D materials.

[1] Lin Niu, Xinfeng Liu, Chunxiao Cong *et al.* "Controlled Synthesis of Organic/Inorganic van der Waals Solid for Tunable Light-matter Interactions", *Advanced Materials*, 2015.

[2] Jiadong Zhou, Qingsehng Zeng, Danhui lv *et al.*, "Controlled Synthesis of High-quality Monolayered a-In_2Se_3 *via* Physical Vapor Deposition", *Nano Letters*, 2015, **15**, 6400.

[3] Chaoliang Tan, Peng Yu, Yanling Hu *et al.*, "High-Yield Exfoliation of Ultrathin Two-Dimensional Ternary Chalcogenide Nanosheets for Highly Sensitive and Selective Fluorescence DNA Sensors", *JACS*, 2015, **137**, 10430.

[4] Fucai Liu, Wai Leong Chow, Xuexia He *et al.*, "Van der Waals p-n Junction Based on Organic-Inorganic Heterostructure", *Advanced Functional Materials*, 2015, **25**, 5865.

[5] Zheng Liu, Matin Amani, Sina Najmaei, PM Ajaya, Jun Lou *et al.*, "Strain and Structure Heterogeneity in MoS_2 Atomic Layers Grown by Chemical Vapor Deposition", *Nature Communications* 2014, **5**, 5246.

[6] Z. Liu, Y. J. Gong *et al.*, "Ultrathin high-temperature oxidation-resistant coatings of hexagonal boron nitride", *Nature Communications*, 2013, **4**, 2541.

[7] S. Najmaei, Z. Liu, W. Zhou *et al.*, "Vapour phase growth and grain boundary structure of molybdenum disulphide atomic layers", *Nature Materials* 2013, **12**, 754–759.

[8] Z. Liu, L. Ma, G. Shi, W. Zhou *et al.*, "In-plane heterostructures of graphene and hexagonal boron nitride with controlled domain sizes", *Nature Nanotechnology* 2013, **8**, 119-24.

Near-field imaging of exciton-plasmon wave functions confined in WS_2 nanotube

Lena Yadgarov[a,b], Michael Mrejen[a], Eitam Vinegrad[b], Ori Cheshnovsky[b], and Haim Suchowski[a]

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Over the last decade vast efforts were devoted to understand and utilize the unique optical properties of van der Waals nanostructures (NS). Great progress in this field was obtained by implying advanced methods for a single-particle characterization. Tenne *et al.*, showed that many layered compounds like WS_2 suffer from inherent instability and are therefore prone to forming closed-cage NS[1]. Recently, it was proposed that WS_2 nanotubes can exhibit strong exciton-plasmon coupling (plexciton) in an *individual* quasi-1D nanotube[2]. Moreover, it was shown that the optical properties of such NS can be controlled by verity of methods[3–4]. Thus, in addition to their application as superior solid lubricants[5], WS_2 nanotubes can be also used for representative case study of fascinating optical phenomena.

Here nano-imaging is used to study the properties of plasmonic and excitonic photo-induced response in an individual WS_2 nanotube in the visible and IR region. The surface waves were detected and imaged in real space in the visible light range using a scattering-type scanning near-field optical microscope (s-SNOM) (Fig. 1). Interestingly, these waves were not observed in the IR range. That finding coincides with the assumption that the plasmon occur manly in the visible region. The standing wave appears with specific incident light polarization and is induced by interference between the tip-excited wave and its reflection from the nanotube.

This study introduces novel approach toward understanding and thus control over a unique physical phenomenon. Previously, only plasmon or phonon-exciton (polariton) interactions in metallic or semiconductor NS were studied using similar technique. Namely, interactions induced by exciton-plasmon coupling have never been explored previously in a single nanotube (or nanowire). The possibility of generating plexciton modes which vary in their wave properties by changes in photo-induced energy could be of high importance for nanophotonic circuitry, saturable absorbers in a mode-locked laser, optical tracking during medical diagnostics (or drug delivery) and more.

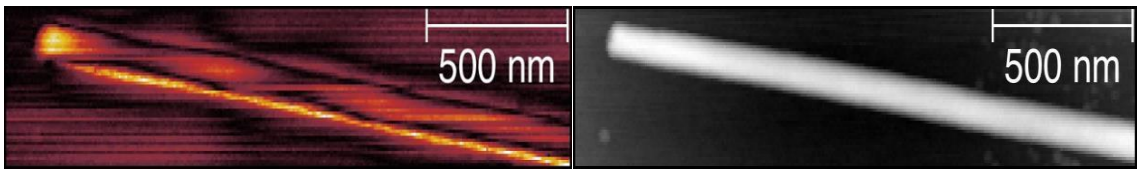

Figure 1 (Left) Plot of the near-field scattering intensity spectra along a representative WS_2 nanotube on a silica substrate. The standing wave can be clearly observed. (Right) Topography image of the same nanotube obtained using atomic force microscopy.

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Electric-double-layer field-effect transistors using polyethylene-oxide cesium perchlorate on two-dimensional materials

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Two-dimensional materials are being widely developed for applications in electronics[1]. High performance devices require technologies for ohmic contacts, p-n junctions, and gate stacks and these are still at a primitive stage of development relative to industry. In this presentation we will review development of electric-double-layer (EDL) doping technology for transistors. Mobile ions in polyethylene-oxide have been shown to be highly effective in forming electric double layers (EDL) in two-dimensional materials[2,3]. Record low contact resistance and high current densities are now demonstrated in WSe_2 and MoS_2 field-effect transistors (FETs)[4]. Highly ideal p-n junctions have now also been demonstrated paving the way for EDL tunnel FETs[5]. This talk will outline the physics and applications of this approach in the development of low-voltage energy-efficient transistors.

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Flexible TFTs and circuits based on monolayer MoS_2

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Mono-layer MoS_2, consisting of only three layers of atoms, could sustain high tensile strain up to 11% in experiment. The ultrathin thickness also guarantees high flexibility. It has much higher carrier mobility comparing to other common used flexible semiconducting material like a-Si or organic material, therefore, MoS_2 has the advantage to achieve high performance flexible electronics. We have fabricated thin film transistors based on single layer CVD-MoS_2 on thin polyimide substrate. Parylene C, a pinhole-free conformal polymer coating, has been used as the insulating layer instead of other brittle oxide dielectric material. With ultrathin polyimide substrate, MoS_2 TFTs are able to sustain small bending radius down to 0.625 mm with only minor variation in performance. Basic circuit units like inverters and ring oscillators are also realized on flexible polyimide substrate. Inverters with high gain value of 9.66 were measured. With the proof of successfully fabricated single flexible TFTs device as well as the basic circuit units, this research shows the feasibility and the potential of the application of MoS_2 in flexible electronics.

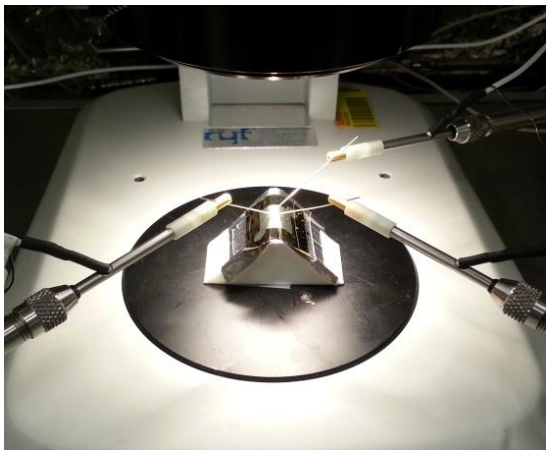

Figure 1 Flexible devices measured on bending stage.

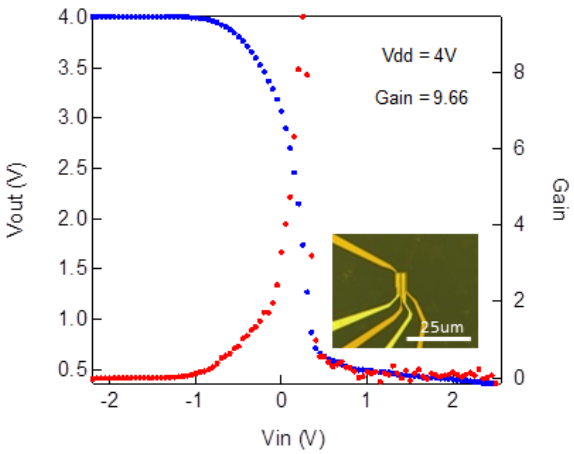

Figure 2 Output characteristics of MoS_2 inverters on flexible polyimide.

How to make monolayer-rich liquid-exfoliated 2D materials suitable for fundamental studies

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In order for 2D materials beyond graphene to be used, large quantities of controlled sizes need to be made available. This can be achieved by liquid exfoliation (LPE) which is particularly appealing because it allows for further solution processing (*e. g.* printing) and composite formation. However, the polydispersity in terms of size and thickness is currently a bottleneck and difficult to control. This is mostly because size and thickness measurements by statistical microscopy are tedious and time consuming and no techniques to easily measure nanosheet sizes, thicknesses, etc., are available.

I will review our recent progress on producing various liquid-exfoliated 2D nanosheets[1]. I will show that nanosheet size, thickness and monolayer content can be quantitatively determined from optical spectroscopy. For example, mean number of layers and lateral dimensions of liquid exfoliated TMDs can simultaneously be obtained from an optical extinction spectrum due to edge and confinement effects[2,3]. Further metrics based on the measurement of the Raman and photoluminescence in liquids can be used to quantify the monolayer (ML) content[3]. This laid the foundation to design centrifugation cascades that can be tailored to specific needs. For example, the monolayer (ML) volume fraction can be increased up to 75%. Such samples are ideal to study the impact of nanosheet size and thickness both in applications and with respect to fundamental optical properties such as absorbance and photoluminescence. The optical measurements (for example narrow PL linewidth) confirm the high structural quality of the liquid exfoliated nanosheets. Such samples are also ideal for further studies into chemical doping of the nanosheets[4].

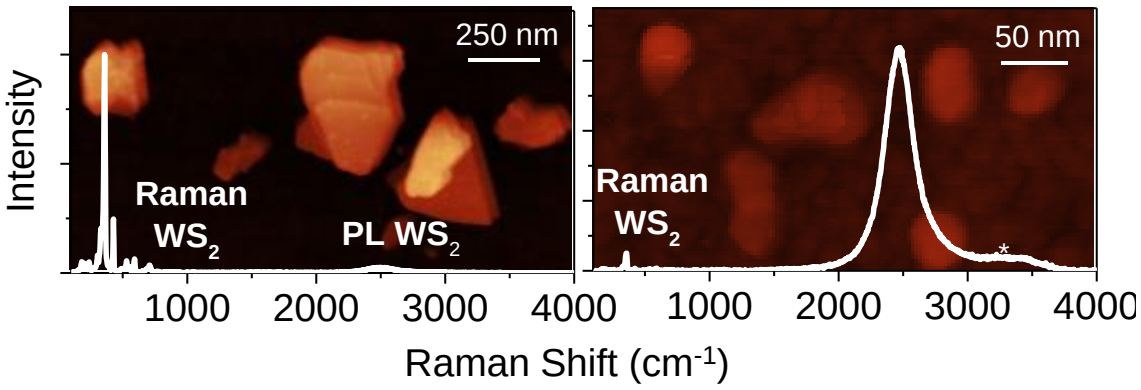

Figure 1 Raman/photoluminescence spectra and AFM images of large, thick LPE WS_2 (left) and monolayer-rich WS_2 (right).

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Top-down and bottom-up routes to solution processable nanosheets: size control, doping, and applications

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Solution phase routes to 2D materials are attractive due to their potential scalability and compatibility with established processing techniques. We have investigated both bottom-up and top-down routes to MoS_2 nanosheets[1–3].

We recently demonstrated that hot-injection of the single source molecular precursor $Mo_2O_2S_2(S_2COEt)_2$ into oleylamine leads to the growth of monolayer MoS_2 nanosheets with small lateral dimensions[2]. Size-control is possible through selection of the reaction temperature. The MoS_2 sheets produced were combined with graphene and used as supercapacitor electrodes, achieving a specific capacitance of 50 mF cm^{-2}[1].

We have used liquid phase exfoliation (LPE) as a simple route to MoS_2 inks[2,4]. We have demonstrated that untreated molybdenite ores can be directly exfoliated in NMP[2]. The solution processability of nano-inks produced by LPE has allowed us to fabricate devices by inkjet printing[4]. Our interest in LPE of nanosheets extends beyond MoS_2, we have recently exfoliated a number of novel 2D materials including SnS, and black phosphorus (BP)[5,6]. BP inks made by LPE have been used to fabricate electrochemical sensors for the cardiovascular disease biomarker myoglobin, demonstrating an extremely low detection limit of 1.4 pg mL^{-1}.

We have also developed a new route to nanosheet inks, combining bottom-up and top-down processing[3]. Aerosol assisted chemical vapour deposition using single source precursors can deposit thin films of layered transition metal dichalcogenides, it is relatively simple to incorporate dopant atoms into the structure during this process. The resulting thin films can then be subjected to LPE to produce suspensions of doped MoS_2 nanosheets[3]. The versatility of single source precursor chemistry means that a wide range of novel, doped transition metal chalcogenides can be accessed by this serial processing route.

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CVD growth of two-dimensional MoS_2 and heterostructures with graphene

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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.

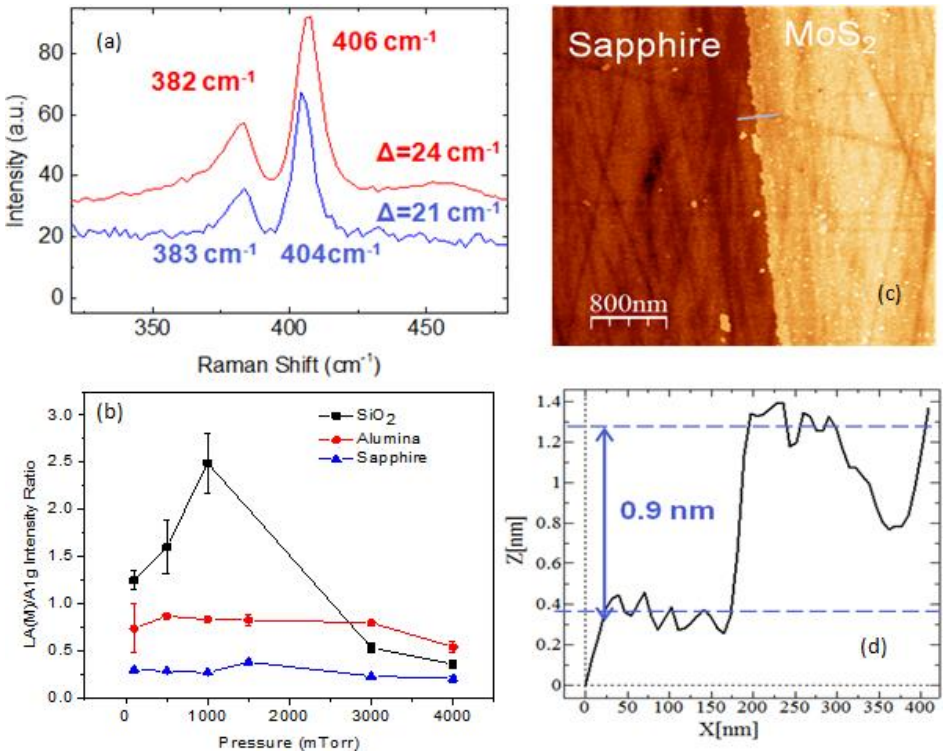

Figure 1 (a) Raman spectrum of CVD deposited MoS_2. (b) LA(M)/A1g peak ratio of deposited MoS_2 on different substrates. (c,d) AFM analysis of obtained films.

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Noble metal transition metal dichalcogenides

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Besides graphene, many more two-dimensional crystals have been discovered or predicted[1–3]. One particularly interesting class are transition metal chalcogenides, whose prototypic material MoS_2 serves as true alternative in 2D electronics[4]. It was shown that quantum confinement effects are very strong in these materials[5]. Here, we present a particularly striking example of quantum confinement: We have recently investigated the performance of noble metal dichalcogenides, *i. e.* PdS_2 and PtS_2[6]. The structure of PdS_2 is still debated, but if stabilized in T-symmetry, it is semiconducting as monolayer, but conducting as bilayer. This suggests that a field effect transistor can be made of a single material, that is, with T-PdS_2 bilayers as electrodes and T-PdS_2 monolayers as channel (Figure 1). Such setup has the potential to lower the contact resistant significantly, leading to low-power electronic applications[7].

Further, I will present first cases of 2D topological insulators containing noble metals.

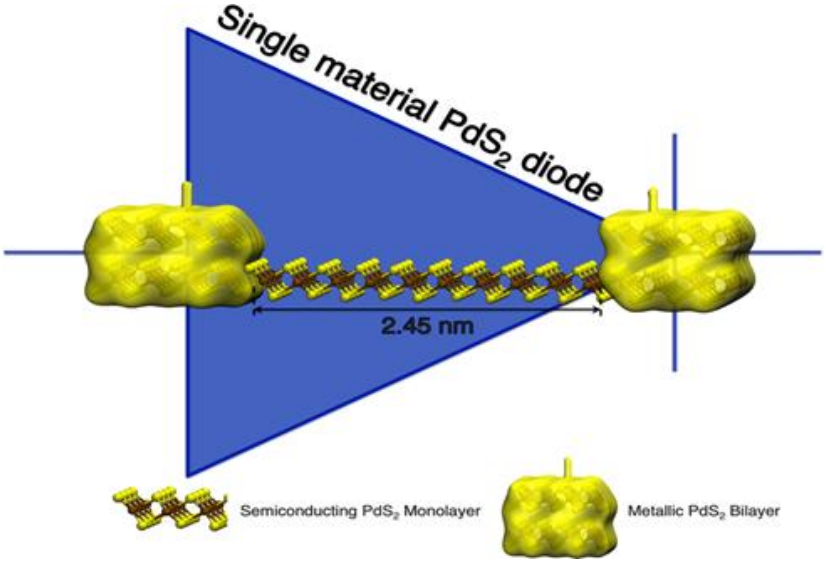

Figure 1 Schematic view of an all-PdS_2 logical junction.

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Determination of length from scattering spectra of liquid exfoliated layered double hydroxides and their use for electrochemical applications

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In this work we describe an easy way to exfoliate nickel hydroxide ($Ni(OH)_2$), cobalt hydroxide ($Co(OH)_2$), magnesium hydroxide ($Mg(OH)_2$), and zinc hydroxide through liquid phase exfoliation in surfactant solution. Through this method we have successfully optimised the production of 2D nanosheets and by examining the effect flake size has on scattering spectra we have shown a relationship between flake length and scattering exponent. This method of determining flake length from the scattering spectra was also applied to many other materials including graphene and boron nitride. Layered double hydroxides (LDHs) are a family of layered materials that show great promise for many electrochemical based applications such as a supercapacitor where we report capacitances of over 800 F/g for $Ni(OH)_2$ and as catalysts in the oxygen evolution reaction (OER) with overpotentials in the range of 200–300 mV when polarised at 10 mA/cm^2 for both $Ni(OH)_2$ and $Co(OH)_2$.

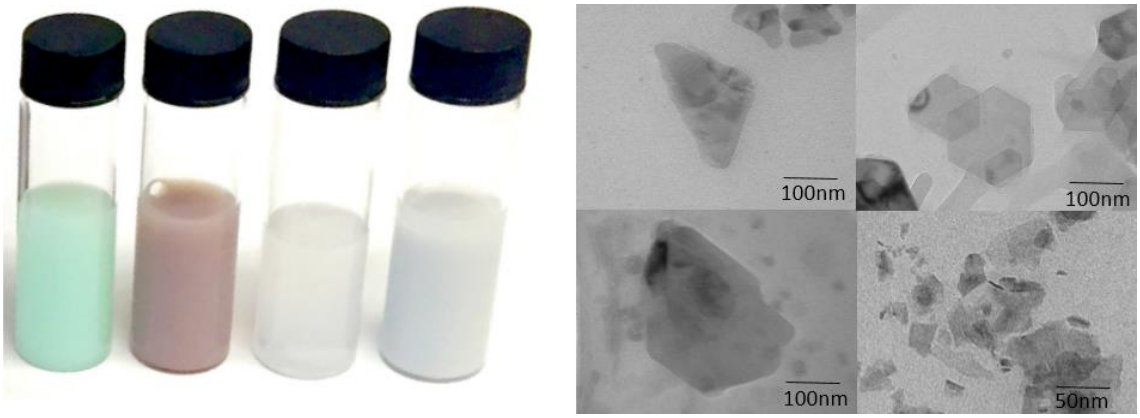

Figure 1 A) Dispersions of $Ni(OH)_2$, $Co(OH)_2$, $Mg(OH)_2$, and $Zn(OH)_2$ exfoliated using the sampling conditions. B) Representative TEM image of $Ni(OH)_2$ (top right), $Co(OH)_2$ (top left), $Mg(OH)_2$ (bottom right) and $Zn(OH)_2$ (bottom left).

Photo-thermionic effect in graphene-based heterostructures

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Conventional photodetectors and solar cells based on semiconductors (or metal/semiconductor interfaces) suffer from two important performance limitations: i) they are insensitive to photons with energies lower than the bandgap (or Schottky barrier height), and ii) the excess photon energy is converted into thermal energy and considered as loss. Here we introduce and experimentally demonstrate a novel way of detecting and harvesting light which overcomes both issues: the photo-thermionic (PTI) effect[1]. This mechanism exploits the unique thermal processes in graphene compared to metal, and profit from the vertical extraction of carriers enabled by the van der Waals (vdW) heterostructure geometry.

Graphene-based vdW heterostructures have already been demonstrated as fast and efficient photodetectors for visible light[2,3], and vertical transistors[4]. Here, we show near-infrared photoresponse in graphene/WSe_2/graphene heterostructures. Due to strong electron-electron interactions in graphene, excess energy is redistributed among other carriers leading to the build-up of a thermalized distribution of so-called hot electrons. This enables a significant fraction of carriers to be injected over the energy barrier at the graphene/WSe_2 planar interface, thus generating a photocurrent. We study this effect over a wide range of optical (wavelength, power, time delay) and electrical (bias voltage, gate voltage) parameters, and obtain good quantitative agreement with a model based on Landauer formalism. From these results, we identify clear strategies for optimizing the efficiency of the PTI effect. This opens up a promising avenue for optoelectronic applications that require sub-bandgap photodetection, size-scalable active area, electrical tunability, broadband and ultrafast response.

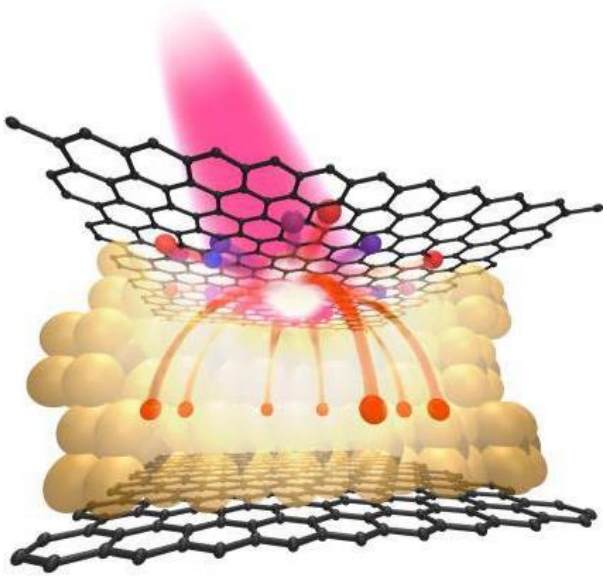

Figure 1 Artistic view of the PTI effect in our graphene/WSe_2/graphene device.

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Magneto-optical properties of individual perovskite nanocrystal

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[b]*Institute of Inorganic Chemistry, ETH, Zurich, Switzerland*
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This work presents magneto-optical characterizations of novel inorganic cesium lead halide $CsPbBr_3$ perovskites, prepared by colloidal synthesis[1]. The induced strong spin-orbit coupling (SOC), together with an inversion-symmetry breaking are the basic conditions to lift the spin degeneracy *via* the so-called Rashba effect[2]. The current work describes the investigation of $CsPbBr_3$ single colloidal nanocrystals, revealing the unique physical phenomena, and in particular the occurrence of a Rashba split.

The sample was prepared by drop cast of $CsPbBr_3$ on top of Si/SiO_2 substrate and placed in confocal microscope, which enables a sub-micron resolution of detected polarized photoluminescence (μ-PL) in presence of a magnetic field, up to 8 T. The microscope was inserted into auto-cooled He cryostat.

The spectra from individual NCs compared to that of ensemble is characterized by sharp bands, with full width half maximum <1 meV, and presence of weak subsidiary bands. The subsidiary bands are shifted away from the main band by several meV, and can be correlated with a vibration modes. By applying a magnetic field the main emission band, as well as the subsidiary bands, were split up to 1.2 meV at 8 T. Further, using linear polarizer at the detection, the non-polarized split bands at 8 T, were found to comprise of two orthogonal linear polarizations.

Under circular polarization detection the main split band and its subsidiary bands are correlated similarly to these of the linear polarization. But the degree of the circular polarization of each split band is not absolute. The co-existence of both linear and circular polarization of the same optical transitions further supports the presence of an elliptical polarization.

The experiments resolve discrete linear and circular polarized narrow excitonic transitions at different magnetic fields. The exciton transitions were accompanied by clear existence of phonon-assisted replica presumably associated with the indirect transitions of the split Rashba bands.

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2D materials: macroscopic and nanoscopic viewpoint

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2D materials are investigated for more than almost a century. Commercial applications of these materials as *e. g.* solid lubricants are known since more than 70 years. A brief historical perspectives will be presented, emphasizing research in transport, optical and the photoelectrochemical properties of 2D materials. The early studies of nanoparticles of 2D materials will be delineated as well. In the second part of the review presentation, the state of the art in research and application of fullerene-like (IF) nanoparticles and nanotubes (INT) from 2D materials will be presented. Advancement in the synthesis and characterization of IF/INT from binary and ternary compounds will be presented. The great progress in the large scale applications of IF and INT from WS_2 and MoS_2 will be presented as well.

Boron nitride encapsulated MoS_2 photodetectors with 1T/1T'-MoS_2 electrodes

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MoS_2 is a semiconductor with a direct band-gap ~1.9 eV in single layer form[1]. Transistors and photodetectors made with MoS_2 as the conducting channel, show high on-off ratio, moderate mobilities and ultra-high responsivities[2,3]. Nevertheless, like in the case of graphene, the device performance is strongly dependent from the environment and the substrate as well as from the quality of the contacts. Encapsulated MoS_2 devices with graphene contacts exhibit superior characteristics, but the fabrication of these devices is more complicated[4]. In our work we explore the encapsulation of single layer MoS_2 with boron nitride in addition to 1T/1T'-MoS_2 side contacts. With this method we plan to improve the carrier transport and the contact resistance of the devices without the use of graphene to side contact the MoS_2 channel. Moreover, by choosing the right thickness of the top boron nitride layer, the photocurrent and the performance of a photodetector can be further enhanced.

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X-ray photoelectron spectroscopy study of the reversible functionalisation of MoS_2

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Transition metal dichalcogenides (TMDs), primarily MoS_2, have become a popular research subject in (opto-)electronics, medicine, electrochemistry and catalysis. In order to tailor the properties of MoS_2 for different applications, the development of functionalisation methods is a high priority. However, due to the relative inertness of pristine, thermodynamically stable 2H-MoS_2 harsh chemical treatments are generally required to induce any covalent bonds. Inspired by work on liquid exfoliated MoS_2[1], we have achieved reversible functionalisation of both CVD-grown monolayers and vapour-grown MoS_2 polycrystalline films, through the use of organic metal carboxylates. Evidence for this functionalisation approach comes mostly from X-ray photoelectron spectroscopy (XPS), which shows the emergence of a new and significant component in the S 2p spectrum at a 6.5 eV higher binding energy than the sulphur in MoS_2 as well as a changing of the Mo 3d spectrum after functionalisation. This reaction can be reversed with acidic treatment restoring the XPS spectra to their original form. It is notable that this entire process was achieved on the semiconducting, thermodynamically stable, 2H-polytype of MoS_2, whereas most previously reported covalent functionalisation of CVD MoS_2 has only been possible on the metallic and unstable 1T-polytype. Secondly we showed that large area polycrystalline MoS_2 thin films can be treated in the same way. This on-chip method of functionalising monolayer MoS_2 opens up potential device applications *e. g.* gas sensors.

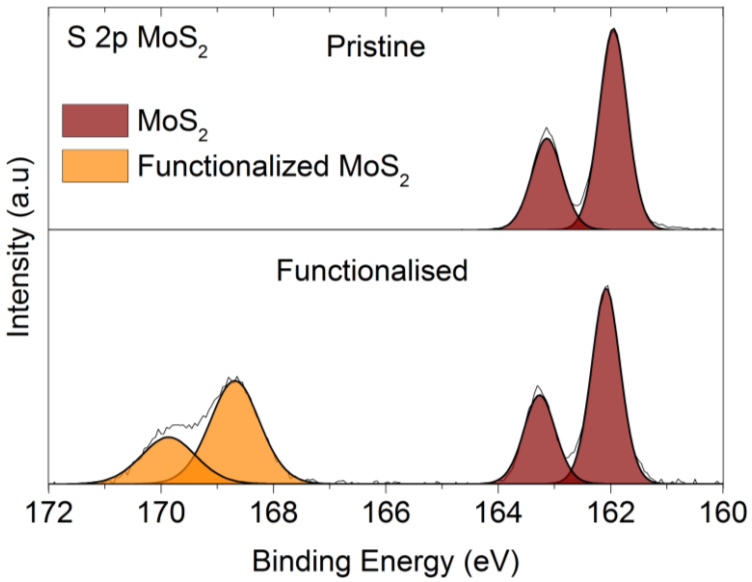

Figure 1 S 2p core level XPS spectra for pristine and functionalised MoS_2.

[1] N. C. Berner, C. Backes *et al.*, *Angew. Chem. Int End.*, **54** (2015), 9, 2638.

Optical Properties of WS_2 Nanotubes

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The recent discovery of localized surface plasmon resonances in inorganic nanotubes and fullerene-like nanoparticles of WS_2 and MoS_2 opened up a new interest in their optical properties[1]. The coexistence of plasmons and excitons in the WS_2 nanotubes leads to their coupling and hybridization. This hybridization makes them a very unique material, since it is the first time this effect was reported in a non-composite system. Techniques such as total extinction, decoupled and transient absorption are used in order to study the carrier dynamics thoroughly.

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Effective chemical approach for single- to multi-layer two-dimensional transition metal chalcogenide nanosheets

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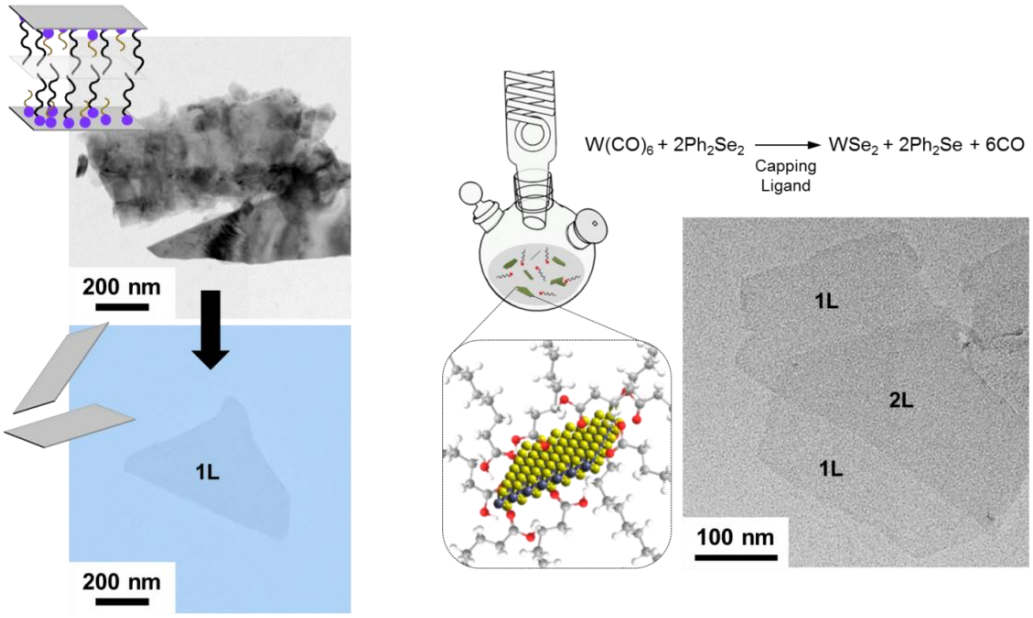
As single- or few-layer two-dimensional (2D) layered transition metal chalcogenides (TMCs) are known to show intriguing properties (*e. g.* direct band gap photoluminescence, high electron mobility, etc.), their preparation methods such as direct synthesis (*e. g.* CVD) and exfoliation from bulk TMCs (*e. g.* dry mechanical cleavages, sonication-assisted solution processes, etc.) have been widely explored. While current methods have their own advantages and drawbacks, there have been clear needs of a simple and effective but yet mild way to obtain high quality TMCs.

In this talk I will discuss the chemical approach for single- to multi-layer nanostructures. Molecular tandem approach for highly effective exfoliation of bulk layered materials and direct chemical synthesis will be discussed. In specific, the new mild and efficient exfoliation method, namely 'tandem molecular intercalation (TMI)' process, utilizes two different Lewis base intercalates. A relatively short molecule acting as a 'primary intercalate' to open the interlayer gaps between TMCs, followed by the longer one, makes randomly mixed bilayers to exfoliate them into the single-layer nanosheets. The bottom-up direct chemical synthetic approach uncovers the new route for the single-layer TMC nanosheets *via* simple reaction parameter control. The kinetics of chalcogen source delivery or binding energy of capping ligands to the reactive edge facets during the crystal growth is found to be key factors to promote exclusive lateral growth modes, which are generally applicable for the formation of single- to multi-layer TMC nanosheets.



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Quantum thermal transport in two-dimensional materials: a NEGF-DFTB study

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Over the last years, two-dimensional materials have attracted considerable interest due to the fact that they offer a new broad playground to explore and develop nanoscale devices with tailored electrical, optical and thermal properties[1]. Recently, many prototypes have been proposed for thermal devices (diodes, transistors, and logic gates) based on graphene[2]. Advanced computational methodologies such a non-equilibrium Green's functions (NEGF) have successfully helped to gain a deep insight into the mechanisms governing their transport properties.

We combine NEGF technique with a density functional tight-binding (DFTB) approach to study the influence of diverse factors on the thermal properties of novel 2D materials. In the ballistic phonon transport regime, we have found out that the effect of ad-atoms and molecular functionalization on the thermal properties of graphene grain boundaries (GBs) sensitively depends on their structural configuration. We have also found an anomalous behavior of the thermal conductance after increasing the uniaxial strain in GBs composed by hBN, Phosphorene, and MoS_2 monolayers, which can be tuned by considering temperature effects in the GB (Fig. 1 and 2).

We also show preliminary results on the influence of many body (phonon-phonon) interactions[3] on the thermal response.

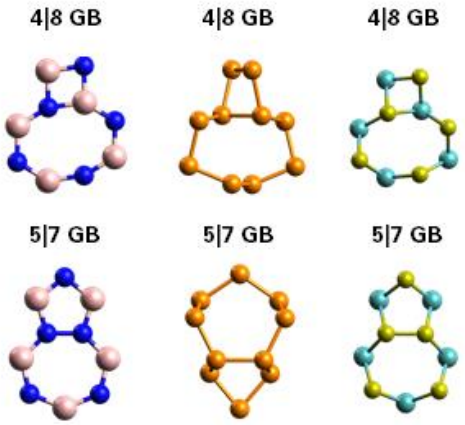

Figure 1 Schematic representations of the grain boundaries (GBs) studied in the present work.

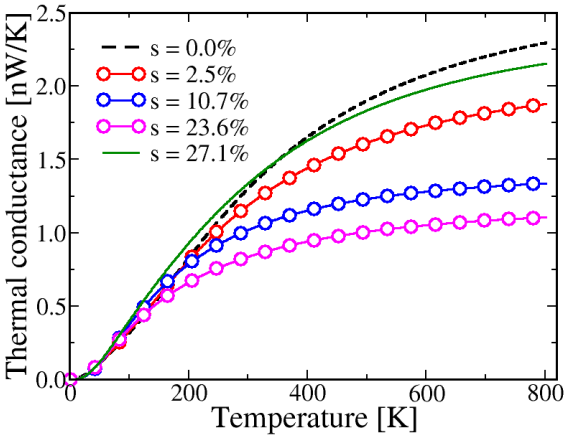

Figure 2 Strain dependence of the thermal conductance for hexagonal boron-nitride 4|8 GB.

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Generation and detection of light in 2D materials and heterostructures

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Two-dimensional (2D) materials are currently receiving a lot of attention for applications in optoelectronics. In this talk, I will review our research activities on electrically driven light emission and photodetection in 2D materials and van der Waals heterostructures. In particular, I will present studies of electroluminescence from MoS_2 and WSe_2 monolayers and their heterojunctions. Further, I will discuss photoconductivity studies of 2D semiconductors, in which we find strong photoconductive gain. We envision that the efficient photon generation and detection, combined with the advantages of 2D semiconductors, such as flexibility, high mechanical stability and low costs of production, could lead to new optoelectronic technologies.

Ehancement of photoluminescence intensity of atomically flat, liquid exfoliated WS_2 monolayers utilizing plasmon excitation

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Among all 2D materials transition metal dichalcogenides (TMD) monolayers form a distinct family of 2D semiconductors with open and direct bandgap holding a promise of new phenomena and novel devices. This renders TMDs an interesting material to study with properties not limited to their extraordinary photoluminescence[1].

Hybrid structures, composed of semiconductors and metallic nanoparticles are a group in which plasmon excitation allows for tailoring the optical response of semiconductors[2]. One of the most interesting effects in these structures is photoluminescence enhancement.

Recent advances on liquid exfoliation of 2D materials and subsequent size selection allows for the preparation of monolayer-enriched dispersions with well-defined size and thickness[3]. Such samples are promising candidates to study optical properties and fabricate composites and hybrid structures due to the possibility of solution processing.

In this work we report the enhancement of PL intensity of liquid exfoliated WS_2 monolayers, coupled with Silver Island Film (SIF). The hybrid structure was prepared by drop-casting WS_2 on SIF, prepared by reduction of silver nitrate with glucose.

To quantify the enhancement and its spectral dependence, WS_2 PL was measured for three excitation wavelengths (405, 485 and 532 nm) on SIF and on glass. In order to collect statistically significant data, 400 emission spectra for each excitation and substrate was acquired by mapping a 200 µm × 200 µm sample region with 10 µm steps. Spatial resolution is 2 µm. The experiment was carried out at temperature of 7 K.

The experiment allowed us to calculate the enhancement factor; it varies between 8, and 22. Spectral dependence of the EF suggests presence of effects beyond excitation rate enhancement – *e. g.* Purcell effect. Significant broadening of PL intensity distribution on SIF is observed, showing significant inhomogeneity of SIF substrate prepared with the described method.

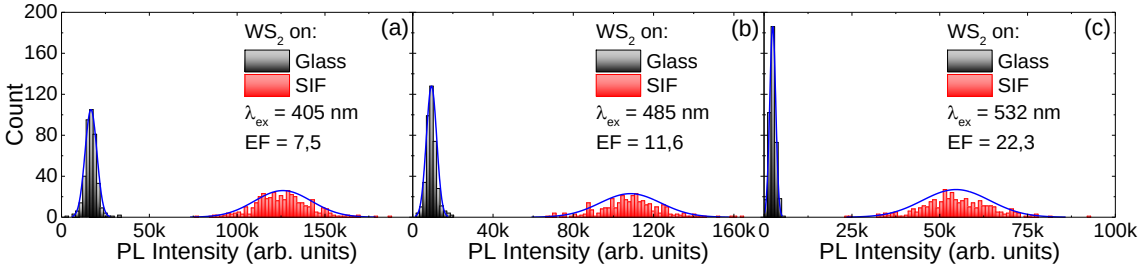

Figure 1 Intensity distributions of monolayer WS_2 PL measured on glass (black bars) and SIF (red bars) for excitation of (a) 405 nm, (b) 485 nm and (c) 532 nm.

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Resonance Raman spectroscopy and excitons in few-layer 2D materials

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Layered crystals such as transition metal dichalcogenides or graphite have attracted great interest, as their monolayer and few-layer forms have distinct physical properties compared to the bulk crystals. These two-dimensional (2D) materials are, on the other hand, very sensitive to their environment, *e. g.* substrates, dielectrics, or other layers of the same material. In this talk we will focus on the optical and vibrational properties of few-layer 2D materials. We will discuss interlayer vibrations arising from optical phonon modes and provide a generalized treatment of these vibrations, allowing predictions of the phonon modes in any few-layer crystal[1,2]. Furthermore, by resonant Raman spectroscopy, we show that these interlayer phonon modes can give information on the spatial extent of the exciton wave functions. Our interpretation is supported by first-principles calculations of the optical properties and exciton wave functions in transition metal dichalcogenides[3].

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High pressure and low temperature Raman scattering in inorganic fullerenes of MoS_2

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Resonance Raman scattering has been widely used to study electronic band structures and to investigate the nature of electron-phonon interactions in semiconductors. A key issue in those studies is the role played by intermediate exciton states. In [1] we demonstrated how Raman scattering of Stokes and anti-Stokes Raman spectra of bulk 2H-MoS_2 is resonantly tuned by pressure and temperature – shifting of the exciton energies, towards that of the exciting laser. Here we extend our study to inorganic fullerenes (IF) of MoS_2[2] and find fundamentally different behavior: no resonant dependence is detected.

Limits on the use of excitons as intermediate state in the scattering process concern, among other aspects, their lifetime. We attribute the different behavior to structural effects that reduce the exciton lifetime: the relative abundance of defects and the random nature of the trigonal prismatic MoS_2 layers[3].

We will present the pressure and temperature dependent Raman scattering and compare the resonant response of the IF system to that of the bulk of 2H-MoS_2[4]. The effect of structural damage on the Raman spectra, as is presented in Figure 1, will also be discussed.

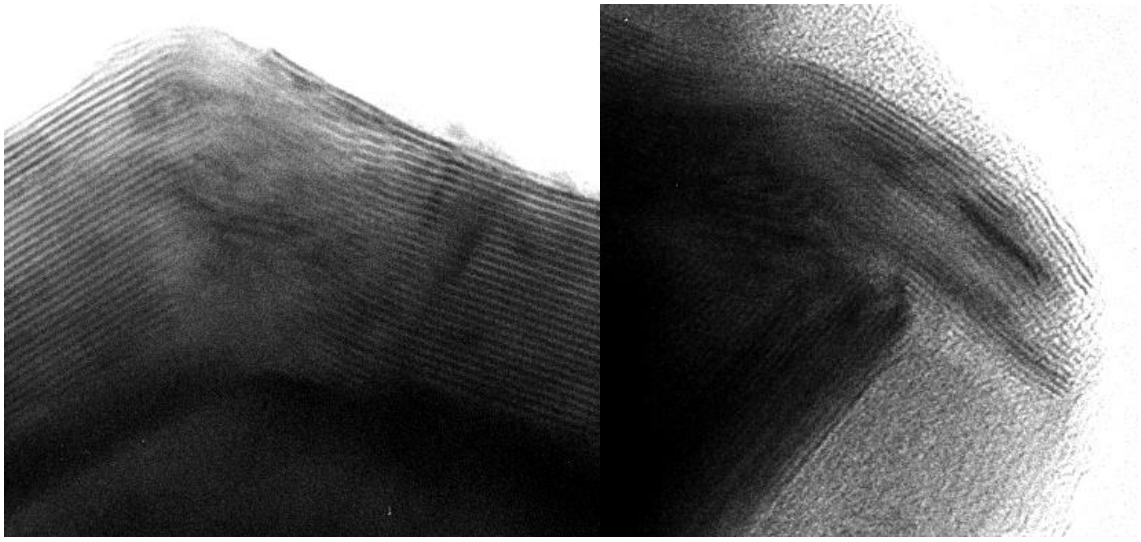

Figure 1 HRTEM of 80 nm diameters IF-MoS_2 particles before (left) and after (right) being released from hydrostatic pressure of 12 GPa.

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Ultrafast optical response of single-layer MoS_2

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In layered semiconductors, such as transition metal dichalcogenides (TMD), the electron-electron interaction is strongly enhanced by both quantum confinement and reduced screening[1]. Furthermore, in these materials the valley polarization can be optically controlled by means of circularly polarized light[2]. We investigate exfoliated single-layer MoS_2 (1L-MoS_2) with ultrafast transient absorption spectroscopy (Fig. 1a) combined with time resolved ab-initio simulations[3] based on the non-equilibrium Green's functions and density-functional theory. This comparison indicates that the non-equilibrium optical properties of TMDs are influenced by the renormalisation of both band gap and exciton binding energies caused by photo-excited charge carriers. The exciton valley relaxation dynamics is investigated by time-resolved Faraday rotation[4]. A circularly polarized pump pulse creates a spin and valley polarized population in the conduction/valence band, which causes the rotation of the linear polarization of a delayed probe pulse. The probe pulse energy is tuned below the absorption gap to be sensitive only to the helicity-dependent light scattering of the photoexcited electrons and holes. Since probe photons couple to the charge carriers orbital momentum, which in 1L-MoS_2 is locked to the valley index, the rotation angle θ_F probes the intervalley relaxation processes. We observe a double exponential decay (Fig. 1b), with an initial fast (~200 fs) decay due to scattering of spin-polarized excitons from K to K'. This is in good agreement with the time scale predicted by the Maialle-Silva-Sham electron/hole exchange interaction mechanism, which can be interpreted as a virtual annihilation of a bright exciton in one valley followed by the creation of an exciton in the opposite valley.

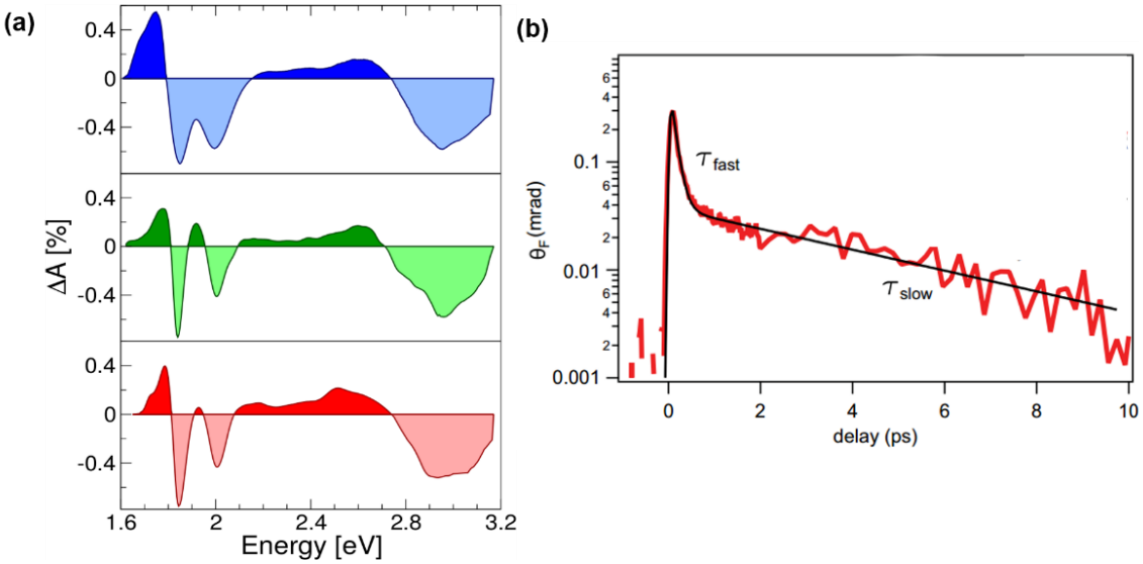

Figure 1 Non-equilibrium optical properties of 1L-MoS_2. (a) Transient absorption spectra (ΔA) at different excitation energies. (b) Time-resolved Faraday rotation.

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Developing a method to calculate response properties for two-dimensional materials in the BAND program

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Predicting optical properties with the help of time-dependent density-functional theory as response properties is a well known task for three-dimensional compounds[1–3] and can already be conducted with many programs. The results can be used to support groups, conducting experimental studies, investigating and developing new materials with optimized functionality.

At the moment, the calculation of response properties for two-dimensional materials can only be achieved using the slab approach, which relies on formalisms for three-dimensional systems. The aim of this project is the formulation and implementation of an algorithm which allows the calculation of response properties for „real" two-dimensional systems.

Here, the main property is the induced density $\delta\rho$. According to equation (1) it depends on the occupied and virtual crystal orbitals $\psi_{i\boldsymbol{k}}$ and $\psi_{a\boldsymbol{k}}$ of the unperturbed system for each point $\boldsymbol{k}$ in reciprocal space, as well as their occupation numbers f and eigenvalues ϵ, and the perturbing field $\boldsymbol{E}$ with the frequency ω. Due to the induced density there exists an induced, effective potential δv_{eff}, representing the change of the Coulomb potential, as well as the change of the exchange and correlation potential. The effective potential and the induced density have to be optimized self-consistently:

$$\delta\rho(\boldsymbol{E},\boldsymbol{r},\omega) = \frac{1}{V_{\text{IBZ}}}\sum_i^{\text{occ}}\sum_a^{\text{vir}}\int_{\text{IBZ}}\psi^*_{i\boldsymbol{k}}(\boldsymbol{r})\psi_{a\boldsymbol{k}}(\boldsymbol{r})\times\frac{(f_{i\boldsymbol{k}}-f_{a\boldsymbol{k}})\int_{\text{UC}}\psi^*_{i\boldsymbol{k}}(\boldsymbol{r}')\left(\frac{i}{\omega}\boldsymbol{j}\boldsymbol{E}+\delta v_{\text{eff}}(r',\boldsymbol{\omega})\right)\psi_{a\boldsymbol{k}}(\boldsymbol{r}')d\boldsymbol{r}'}{(\epsilon_{i\boldsymbol{k}}-\epsilon_{a\boldsymbol{k}})+\omega+i\eta}d\boldsymbol{k}+c.c.(-\omega). \quad (1)$$

To enhance the performance of the new implementation this equation is implemented in a Bloch basis function representation instead of the crystal orbital representation. Hence, the sparseness of the necessary, intermediate matrices can be used to reduce the computational effort.

For the integration in reciprocal space the improper integrals $\int_{\text{IBZ}}\frac{1}{(\epsilon_{i\boldsymbol{k}}-\epsilon_{a\boldsymbol{k}})+\omega+i\eta}d\boldsymbol{k}$ that needed to calculate the integration weights, can now be evaluated by means of an analytical and a numerical approach.

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Function design *via* organization of 2D oxide nanosheets at nano- to mesoscale

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We have successfully synthesized a variety of 2D metal oxides nanosheets with useful properties. Precursor layered compounds were exfoliated into monodisperse single layers *via* hydration-driven massive swelling in aqueous amine solutions[1]. Accordingly we have applied solution-based processes to organize colloidal nanosheets at nano- to mesoscale. Electrostatic self-assembly or Langmuir-Blodgett deposition allowed to organize them layer-by-layer into well-controlled lamellar nanostructures including heteroassemblies[2,3]. On the basis of this approach, we developed various nanofilms showing advanced functionalities, *e. g.* superior dielectric/ferroelectric properties and photochemical activities. On the other hand, we found that novel mesoscopic structures were formed through the swelling of layered crystals or alignment of oxide nanosheets under high magnetic field[4,5]. The intersheet separation could be varied from several nm to over 100 nm by controlling the electrolyte concentrations. Furthermore, the mesostructures in aqueous media were fixed by turning the systems into a hydrogel, which was attained *via* addition of some vinyl monomer followed by its UV-assisted polymerization. The obtained hydrogels exhibited unique optical and mechanical properties.

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Electrostatic design of the electronic properties of 2D materials

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Collective electrostatic effects are well known to crucially determine the electronic properties of metal-organic interfaces[1]. Exploiting these effects and relying on quantum-mechanical simulations, we have recently suggested to develop a toolbox that allows the realization interfacial quantum-cascades and quantum-well structures[2], a direction in which first experimental steps have already been undertaken[3].

The present contribution focuses on extending the concept of electrostatic materials design to low-dimensional systems like graphene and hexagonal boron-nitride[4]. Employing density-functional theory based band-structure calculations we show how collective electrostatic effects can be exploited to modify the energy landscape of prototypical 2D materials. They can be used to localize states in specific regions of space and to efficiently control their energies. This can be achieved either by directly manipulating the 2D material or by the adsorption of suitably designed multipolar organic molecules. This also allows controlling the character of specific bands. In graphene the achievable effects are diminished by electrostatic screening effects, while they remain large in hexagonal boron-nitride or molybdenum-disulfide.

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Thermally assisted conversion – a versatile route for the synthesis of transition metal dichalcogenides

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Two-dimensional transition metal dichalcogenides (TMDs) have moved to the foreground of the research community owing to their fascinating properties which make them of great interest for both fundamental studies and emerging applications. While TMDs possess attractive properties, their synthesis in a scalable and reproducible manner remains a challenge. Thermally assisted conversion (TAC) of predeposited transition metal films is a method which shows promise for the industry-compatible synthesis of these materials[1,2]. The potential of TAC derived TMDs for various applications in the realm of electronics and energy will be discussed. The fabrication of high-performance gas sensors, consisting of MoS_2 channels, with room-temperature detection limits in the ppb range for NH_3[3] and large-scale heterojunction diodes, formed by transferring n-type MoS_2 onto p-type Si, will be outlined[4].

Beyond commonly reported TMDs, the synthesis of late transition metal dichalcogenides using this methodology, in particular $PtSe_2$, will be detailed. This exciting new material is characterised extensively and its Raman characteristics elucidated[5]. Its use as the active component in a variety of devices, which is enabled by the facile and scalable synthesis afforded by TAC, will be outlined.

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Uniaxial compression in monolayer MoS_2 and WS_2

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Strain engineering of electronic structure of TMDCs has become the focus of many studies. While this topic has been explored from a plethora of various theoretical angles, however, only a few experimental works exist for MoS_2 and fewer yet for WS_2. The existing ones focus mostly either on axial tension or hydrostatic pressure. However, axial compression – both in-plane and out-of-plane – offers additional treats.

The direct out-of-plane compression was conducted in an anvil cell without pressure transmitting medium, the in-plane compression using a cantilever beam bending device with PMMA as a support and thin parylene layer as the cover. The behaviour of 1L MoS_2 and WS_2 was compared to 2L and bulk, by in-situ monitoring of the strain-induced changes by Raman spectroscopy and photoluminescence (PL). The experimental study was accompanied by theoretical calculations of the band structure in a very detailed sequence of steps, as well as by calculations of the electron localization function.

In the case of out-of-plane compression, the Raman and PL data are in an excellent agreement with the theoretical results: the changes of the electronic structure indeed require only small axial pressures, namely ~0.5 GPa to induce the direct-indirect band-gap semiconductor transition, and ~3 GPa to reach the semimetallic state in 1L MoS_2[1] and similar values for 1L WS_2. The comparison, both experimental and theoretical, to hydrostatic pressure and to the bulk also reveals the major differences in the impact of the pressure type on the individual structural parameters of the crystal lattices.

In the case of in-plane compression, the effective strain was first calibrated under a tensile experiment (the same setup and sample). In general, the efficiency of interfacial stress transfer is ~50% using PMMA substrate, upon comparison with theoretical calculations, consistently from Raman and PL shifts. As expected, the band gap energy is decreasing under tension and increasing under compression. However, in contrast to the linear evolution of both Raman and PL peaks under tension, the compressive strain is continuously released after reaching about −0.5% level, indicative of a similar buckling failure as previously observed for monolayer graphene embedded in polymer[2].

The work was supported by Czech Science Foundation (project nr. 14-15357S).

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Two-dimensional dipolar exciton fluids

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The advancement of the fabrication capabilities and the quality of atomically thin two-dimensional heterostructures, and the observations of direct and in particular indirect excitons open up possibilities to further explore and expand the rich and exciting physics of interacting exciton quantum fluids, only observed in GaAs-based heterostructures.

In this talk I will review some of the most recent results in dipolar exciton fluids research in GaAs bilayer systems, the standing open questions and challenges, and the opportunities that the new atomically thin materials might have in this context. In particular, I will overview several topics we have looked at over the past few years in GaAs-based materials, including:

1. Many-body effects and collective phenomena of indirect, dipolar excitons, from intricate particle correlations to dipolar quantum liquids and dipolar molecules.

2. Electro-optical devices with long lived dipolar excitons, transport, routing, and dipolar lattices.

3. Interacting dipolar polaritons in optical waveguides devices.

The intention of the talk is to share some of the body of knowledge gained on indirect exciton fluids over the years, and hopefully to spark new research directions and a lively discussion between researchers working on dipolar excitons and polaritons in GaAs systems and those working on new two-dimensional materials.

Mechanism of charge carriers generation in few-layer MoS_2

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Light-matter interaction in the semiconductor MoS_2 forms excitons with binding energy ranging from ~0.1eV (MoS_2 in bulk form) and >0.5 eV (monolayer MoS_2). Despite the huge exciton binding energy an efficient photocurrent generation was observed[1].

To investigate the relaxation dynamic of excitons we used femtosecond optical spectroscopy[2]. We observed that in few-layer MoS_2 hot excitons dissociate into charge carriers during 700 fs. We estimated that around 100% of excitons are converted to charges. An upper limit for lifetime of the photogenerated charge carriers population of 4 ms is obtained from cw photomodulation spectroscopy.

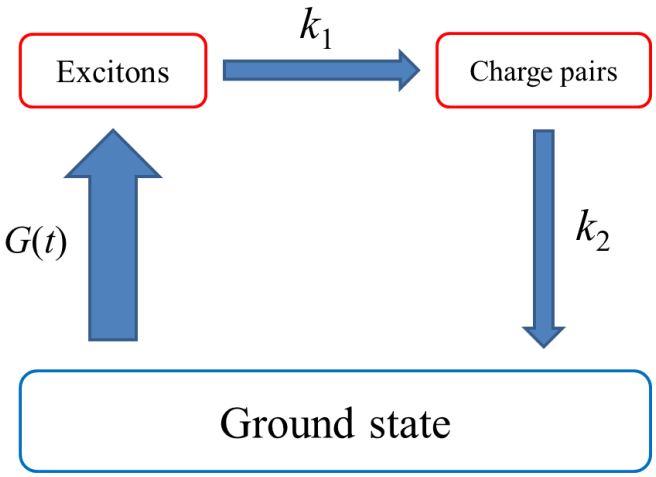

Figure 1 Scheme of excitons dissociation.

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Electro-optical properties of monolayer semiconductors

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Monolayer semiconductors are attractive for realization of unconventional electro-optical devices that rely on strong exciton-mediated light-matter interaction and its electrical control. Here, we discuss electrical excitation and manipulation of excitons in tungsten dichalcogenide monolayers and bilayers. Planar electroluminescence from monolayer semiconductors requires spatially uniform and balanced injection of both electrons and holes into an atomically thin semiconductor layer. The key challenge is to overcome the short resident time of carriers that inhibit efficient formation of excitons. While multiple quantum well structures based on alternating layers of monolayer semiconductors and insulators have proved useful for achieving longer carrier resident time, an improved emission quantum yield is achieved at a cost of high device resistance and a complex device structure. Here we report bright planar electroluminescence from a simple metal-insulator-semiconductor (MIS) diode built entirely from 2D materials. We show, in our graphene-hBN-WS_2 devices, holes in the graphene electrode tunnel into WS_2 through the insulating hBN layer and efficiently recombine with electrons that are present in the WS_2 layer. We further discuss giant Stark effect in monolayer and bilayer WSe_2 samples sandwiched between hBN layers. Our observations indicate that intralayer excitons in these materials are highly robust and remain stable under large electric fields contrary to theoretical predictions.

Relaxation processes of photogenerated charges in MoS_2 and WS_2

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Charge carrier photogeneration in semiconducting transition metal dichalcogenides (TMDs) has been ascribed to dissociation of non-equilibrium excitons. However, the parameters governing this process, as well as the fate of the photogenerated charges are still elusive.

Here, we use femtosecond optical spectroscopy to study the exciton and charge dynamics following impulsive photoexcitation in few-layer WS_2. We confirm excitons as the primary photoexcitation species and find that they dissociate into charge pairs with a time constant of about 1.3 ps. these charges diffuse through the samples and get trapped at defects[1], such as flake edges or grain boundaries, causing an appreciable change of their transient absorption spectra.

We have also performed a systematic study how the charge relaxation dynamics depends on thickness and pump fluence in MoS_2. After exciton dissociation charges diffuse. However, there is a fluence dependent competition between different processes that limit charge diffusion.

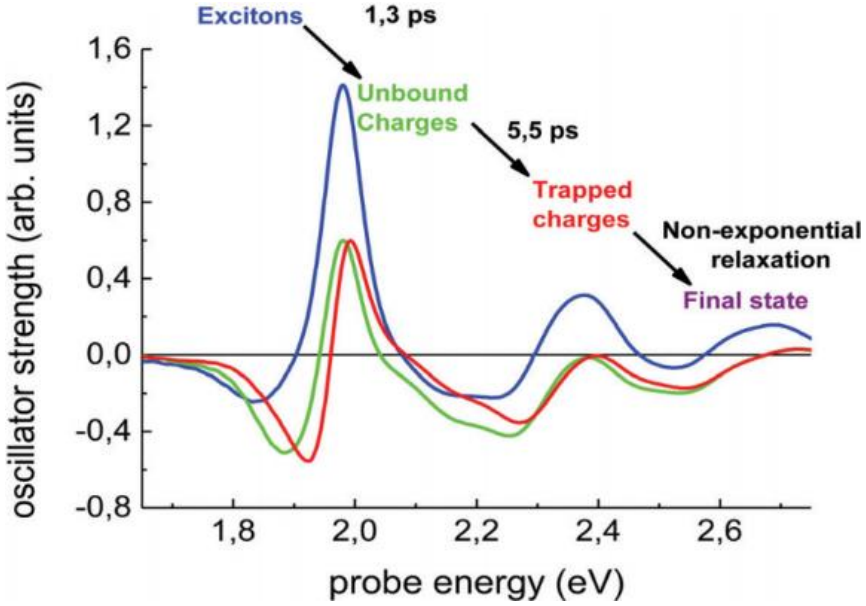

Figure 1 Relaxation ladder of WS_2 photoexcited states.

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Twist-induced tuning of interlayer coupling in monolayer dichalcogenide heterostructures

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Two-dimensional transition-metal dichalcogenides (TMDs) have recently emerged as a promising novel class of semiconducting materials. A fascinating aspect of these two-dimensional crystals is the possibility of constructing functional heterostructures by vertical stacking of different TMDs, and several optoelectronic devices based on this concept have already been demonstrated[1]. In TMD heterostructures, the relative crystallographic orientation of adjacent layers (twist angle) offers a new degree of freedom that can influence the interlayer coupling.

Here, we report on a systematic study of interlayer coupling in heterostructures consisting of different monolayer TMDs by means of optical spectroscopy. The heterostructures are fabricated in a deterministic stacking process and characterized using photoluminescence, second-harmonic generation and Raman microscopy. We demonstrate that a mild post-stacking annealing step reliably leads to strong interlayer coupling, which manifests itself in pronounced interlayer exciton emission and the emergence of an interlayer breathing mode in low-frequency Raman spectra.

We study these signatures of electronic and vibronic interlayer coupling in a large number of heterostructures with well-defined twist angles. Remarkably, we observe a systematic dependence of, both, the interlayer exciton emission energy and the layer breathing mode frequency, on the twist angle. We briefly discuss possible microscopic mechanisms responsible for this twist angle dependence.

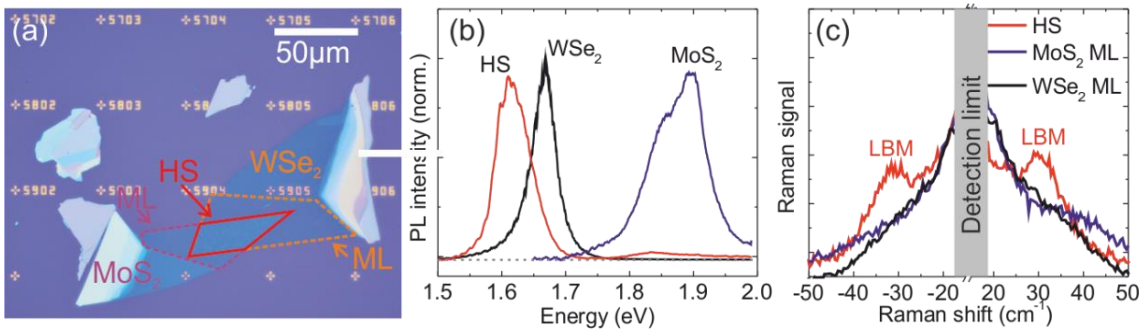

Figure 1 (a) Microscope image of a MoS_2-WSe_2 heterostructure (HS). (b) Photoluminescence spectra of HS and the constituent monolayers. (c) Low-frequency Raman spectra showing layer breathing mode (LBM) in the HS.

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Giant unconventional electroabsorption in monolayer MoS_2

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To translate electrical into optical signals one uses the modulation of either the refractive index or the absorbance of a material by an electric field. Contemporary electroabsorption modulators (EAMs) employ the quantum-confined Stark effect (QCSE)[1–3] the field-induced red-shift and broadening of the strong excitonic absorption resonances characteristic of low-dimensional semiconductor structures. Here we show an unprecedentedly strong transverse electroabsorption (EA) signal in a monolayer of the two-dimensional semiconductor MoS_2. The EA spectrum is dominated by an apparent linewidth broadening of around 15% at a modulated voltage of only $V_{pp} = 0.5$ V. Contrary to the conventional QCSE, the signal increases linearly with the applied field strength and arises from a linear variation of the distance between the strongly overlapping exciton and trion resonances. The achievable modulation depths exceeding 0.1 $dBnm^{-1}$ bear the scope for extremely compact, ultrafast, energy-efficient EAMs for integrated photonics, including on-chip optical communication.

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Processing and applications of liquid-phase exfoliated two-dimensional nanosheets

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Not all crystals form atomic bonds in three dimensions. Layered crystals, for instance, are those that form strong chemical bonds in-plane but display weak out-of-plane bonding. This allows them to be exfoliated into so-called nanosheets, which can be micrometers wide but less than a nanometer thick. Such exfoliation leads to materials with extraordinary values of crystal surface area, in excess of 1000 square meters per gram. This can result in dramatically enhanced surface activity, leading to important applications in microelectronics, energy storage and harvesting, composites, etc. Another result of exfoliation is quantum confinement of electrons in two dimensions, transforming the electron band structure to yield new types of electronic and magnetic materials. Exfoliated materials also have a range of applications in composites as molecularly thin barriers or as reinforcing or conductive fillers. Liquid phase exfoliation has been proved to be a cheap, scalable method for the mass production of 2D sheets[1-4]. This talk will first discuss the galaxy of existent layered materials, with emphasis on synthesis, liquid-phase exfoliation, and characterization, to finish off with some key applications recently developed in our laboratories, ranging from energy storage to composites[5–7].

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Optical properties of WS_2/MoS_2 heterostructures from chemical vapor deposition

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Layer-by-layer stacking or lateral interfacing of atomic monolayers has opened up unprecedented opportunities to engineer two-dimensional (2D) materials[1]. Transition metal dichalcogenide (TMD) heterostructures are particularly interesting for novel optoelectronic and photovoltaic applications due to their optical properties[2]. TMD materials in their monolayer form possess an optical bandgap[3,4] in visible and near infrared spectral range and exhibit strong light-matter interaction. Investigations of optical properties of such heterostructures built on the basis of monolayer TMDs offer a rich collection of information about their physical properties and functionalities.

Realization of TMD heterostructures with mechanically exfoliated monolayer flakes is possible but impractical. On the other hand, fabrication of TMD heterostructures using chemical vapor deposition (CVD) growth is simple and scalable, paving the way for the creation of 2D materials with novel and exciting properties. Here, we report on the optical characterization of WS_2/MoS_2 heterostructures on SiO_2/Si wafers. The vertical heterostructures are verified by Raman and photoluminescence (PL) spectroscopy characterization. Depending on heterostructure geometry, the measurements of absorption, differential reflection and PL spectra in the various area of interest for different stacking angles between the stacked layers provide us with information on exciton peaks evolution due to intralayer or interlayer interactions between WS_2 and MoS_2 layers.

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Tunnelling in van der Waals heterostructures

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When conductive 2D materials (*e. g.* graphene or transition metal dichalcogenides) are separated by an atomically thin insulating 2D crystal, quantum mechanical tunnelling leads to appreciable interlayer current between two 2D conductors due to the overlap of their wavefunctions. These tunnel devices reveal exciting physics and great potential for applications: resonant tunnelling, negative differential conductance, light emission and photovoltaics, to name a few. In this presentation we will outline the current status and perspectives of our work on tunnelling transistors based on 2D materials assembled into van der Waals heterostructures. Particularly, we will present mono- and bilayer graphene tunnelling, tunnelling in 2D crystal-based quantum wells, and tunnelling in superconducting 2D materials. Such effects as momentum and chirality conservation, phonon- and impurity-assisted tunnelling will be reviewed. Finally, we will discuss conceivable practical applications.

A theoretical ride over 2D landscapes

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I will discuss strategies and examples on how to address, from a theoretical and computational standpoint, the description of key properties and processes occurring in different layered materials of deep technological interest (BP, TiS_2, MoS_2, GaS)[1–4].

I will propose comprehensive models for chemical reactivity of layered materials at the nanoscale. Focus will be on exfoliated nanoflakes and the role of ribbon edge structures as important reaction centres, especially relevant for environmental stability of these materials under exposure to water and oxygen. It will be shown how a controlled oxidation of 2D nanoribbons can lead to a fine-tuning of electronic properties in TiS_2, enabling important technological applications in surface catalysis and photovoltaics.

I will illustrate how progress in the understanding of exfoliation, basal plane functionalization and chemical reactivity in this new class of materials can be achieved by adopting a comprehensive and concerted approach, *i. e.* combining multidisciplinary competences of experimental and theoretical research. I will demonstrate how the subtle interplay between many body contributions to the dispersive interactions keeping these materials together, charge polarization, thermodynamics and kinetics of the relevant processes, can only be described using leading edge first principles methodologies based on density functional theory, including van der Waals corrections.

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Electrical transport properties of ReS_2 with polymer electrolyte gating in the high-doping limit

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Two-dimensional (2D) materials have emerged as promising candidates for future electronic applications. Among them, transition metal dichalcogenides (TMDs) demonstrate not only potential as ultrathin transistor channel material, but also intriguing spin and valley physics, which in principle could allow new types of devices and circuits. Here we report on the first study of two-dimensional anisotropic ReS_2 at high doping levels, enabled by polymer electrolyte gating. Significantly increasing the doping level using electrolyte instead of standard solid gate, we measured an unusual modulation of the conductivity at high carrier densities in monolayer ReS_2. In the case of thicker flakes, the effect is milder and an insulator-metal-insulator sequence with increasing doping is observed. Transport measurements provide the evidence of major influence of ionic disorder. Furthermore, we propose a transport model, describing the observed effect.

Electronic properties of 2D transition-metal chalcogenides beyond MoS_2

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Transition-metal chalcogenides (TMC) are widely investigated materials for perspective utilisation in nanoelectronic and optoelectronic devices, especially as 2D systems. The prototypical TMC, MoS_2, in the forms of mono- and multi-layers is already well-known and its electronic properties are well-understood, with direct band gap characteristic of monolayers, giant spin-orbit coupling in non-centrosymmetric systems, or modulations of these properties using strain or external electric field. However, the plethora of 2D TMC materials is very large and many systems exhibit similarly interesting band structure signatures. Among others, we would like to present our results on MX materials (M = Ga, In; X = S, Se, Te) with honey-comb symmetry, showing *e. g.* the effect of quantum confinement on the electronic properties of these layered systems.

The importance of steric effects for interlayer interactions in 2D homo- and heterostructures

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We theoretically and experimentally study interlayer interactions in 2D materials. Dozens of MoS_2 bilayers with well-defined twist angle were measured by stacking single crystal monolayers using ultraclean transfer techniques. It is observed, both by photoluminescence measurements and by angle-resolved photoemission spectroscopy, that continuous changes in the interlayer twist angle lead to strong, continuous tuning of the indirect optical transitions, which implies a change of the band gap up to a maximum of 120 meV at a twist angle of ~40°. Electronic structure calculations are used to show that the tuning of the band gap arises from an increase of the bilayer separation caused by steric repulsion of sulfur atoms[1,2].

A similar analysis of MoS_2/WSe_2 heterostructures leads to comparable, twist angle-dependent changes of the indirect optical transitions, although they are smaller in magnitude. Electronic structure calculations show that these effects are again mostly related to steric effects.

Among various experimental and thoeretical results, this presentation will focus on the importance of steric effects on structural and electronic properties of 2D homo- and heterostructures and discuss them in some detail.

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Morphological manipulation of the luminescent response of atomically thin indium selenide nanosheets

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Many efforts have been devoted to manipulate the morphology of two-dimensional (2D) materials to tune and improve their functionalities. Single layers (SLs) of transition-metal dichalcogenides offer unquestionable technological applications[1–3]. Nevertheless, tuning their properties for optoelectronic applications is challenging due to the intrinsically localized nature and orbital character of the d-states that dominate their valence and conduction bands. 2D forms of other layered semiconductors, as indium selenide (InSe), are less explored and may exhibit interesting and tunable properties[4–6]. First-principles calculations predicted that 2D InSe should produce a band-gap tuning window as large as 1.1 eV[5] and, experimentally, a blue shift of the optical band gap of 0.2 eV has been already observed in 5 nm thick InSe nanosheets[5,6]. Also, devices based on few-layer InSe have shown promising applications[7–9]. In this communication, we show the ability of nanotexturing strategies to enhance the luminescent response of atomically thin InSe nanosheets. Besides, quantum-size confinement effects make InSe to exhibit the largest band gap tunability range observed in a 2D semiconductor. These results are relevant for the design of new optoelectronic devices, including heterostructures of 2D materials with optimized band gap functionalities and in-plane heterojunctions with minimal junction defect density.

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Magnetoconductance oscillations and edge states in semiconducting monolayer transition metal dichalcogenides

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We have developed a **k**·**p** theory framework (see, *e. g.* the recent review in [1]) to describe the dispersion of the conduction and valence bands at their extrema (the K, Q, Γ and M points of the hexagonal Brillouin zone) in semiconducting monolayer transition metal dichalcogenides (TMDCs). We use this theory framework to study a variety of problems. Firstly, motivated by recent experiments[2] that measured the magnetoconductance properties of TMDCs, we investigate how the spin-orbit coupling and the broken valley degeneracy of the Landau levels (LL) affect the Shubnikov-de Haas oscillations in TMDCs[3]. We find that in a wide magnetic field regime the valley degeneracy breaking of the LLs is linear in magnetic field. We use the self-consistent Born approximation and the Kubo-formalism to calculate the Shubnikov-de Haas oscillations of the longitudinal conductivity and compare the results of our theoretical calculations with recent measurements. Secondly, we derived boundary conditions for the bulk **k**·**p** Hamiltonian to describe nanoribbons of monolayer TMDCs[4]. Focusing mainly on zigzag edges, we analyze the edge states and their dispersion relation in MoS_2 in particular, and find good agreement with the results of previous density functional theory calculations. Finally, we briefly discuss the extension of the **k**·**p** theory framework to bilayers of TMDCs.

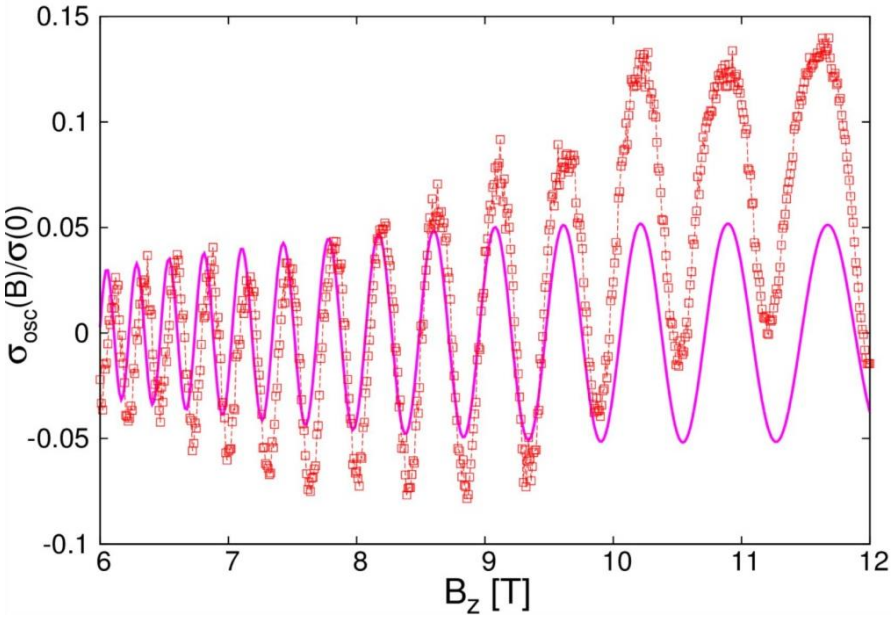

Figure 1 Shubnikov-de Haas oscillations in the magnetoconductance: measurement (squares)[2] and theory (solid lines)[3].

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Ambient intercalation and rapid expansion of MoS_2 crystals

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Intercalation of layered materials is a common exfoliation strategy, since the expanded interplanar distance weakens the van der Waals bonds, easing the separation of layers to nanosheets[1]. But the fact that MoS_2 resists intercalation by all but the strongest reducing agents has limited the protocols to the use of alkali metals. These procedures, however, are inherently dangerous and hard to scale up, since they must take place in a controlled atmosphere devoid of oxygen and water, and lead to chemically altered material[2]. We present a new method of MoS_2 intercalation by organic molecules that takes place at ambient conditions. The intercalated crystals expand rapidly when exposed to a focused electron beam (Fig. 1,2) or heating, behaving similarly to expandable graphite[3]. Besides demonstrating a new type of intercalation and expansion of MoS_2 and possibly other layered materials, our results show that the expanded crystals are a suitable precursor for liquid phase exfoliation.

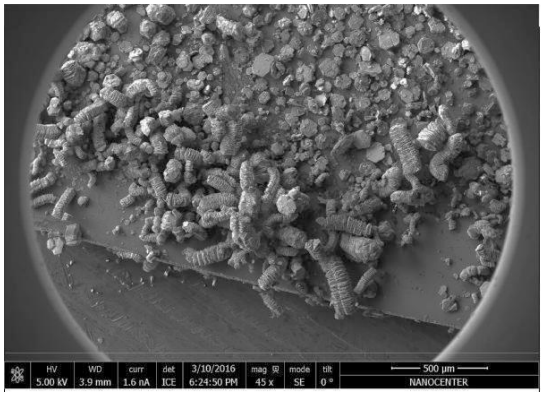

Figure 1 Intercalated MoS_2 crystals expanded by focused electron beam in contrast to unexpanded crystals.

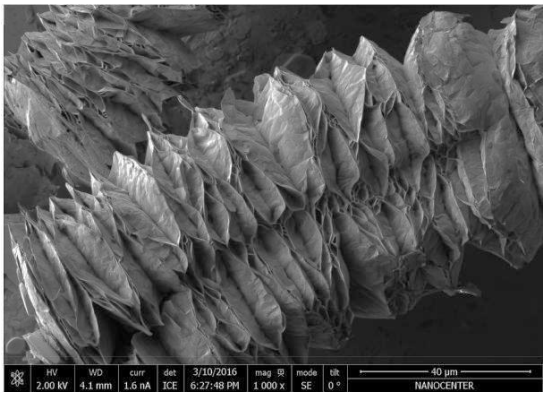

Figure 2 A close-up of one of the expanded crystals shows an accordion structure similar to that of expanded graphite.

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Novel narrow gap 2D semiconductors for optoelectronics and straintronics

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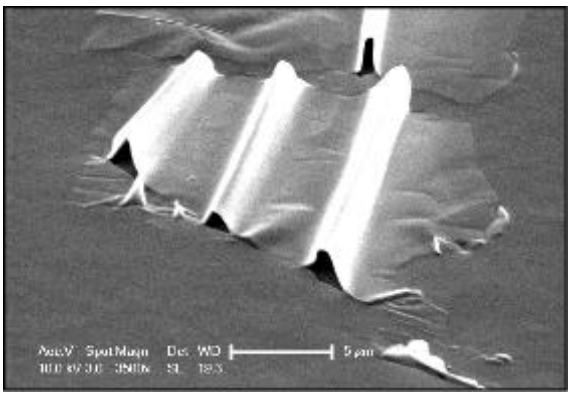
In this talk I will review the recent progress on the application of atomically thin crystals different than graphene on optoelectronic devices. The current research of 2D semiconducting materials has already demonstrated the potential of this family of materials in optoelectronic applications[1–4]. Nonetheless, it has been almost limited to the study of molybdenum- and tungsten-based dichalcogenides (a very small fraction of the 2D semiconductors family). Single layer molybdenum and tungsten chalcogenides present large direct bandgaps (~1.8 eV). Alternative 2D semiconducting materials with smaller direct bandgap would be excellent complements to the molybdenum and tungsten chalcogenides as they could be used for photodetection applications in the near infrared. Furthermore, for applications requiring a large optical absorption it would be desirable to find a family of semiconducting layered materials with direct bandgap even in their multilayer form.

Here I will summarize the recent results on the exploration of novel 2D semiconducting materials for optoelectronic applications: black phosphorus[5–7], TiS_3[8,9]. Recent efforts towards tuning the optoelectronic properties of 2D semiconductors by strain engineering will be also discussed[10,11].



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CVD growth of transition metal diselenides

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Transition metal dichalcogenides (TMDs) in their two-dimensional (2D) monolayer form have attracted extensive attention because of the unique properties that lead to a variety of next generation electrical and optoelectronic device applications. Among them, MoS_2 is the first and most investigated member of TMDs family because of its abundance in nature and quite simple process of synthesis[1]. Whereas, there are numerous reports on MoS_2, the synthesis and characterization of the monolayer selenide TMDs family such as $MoSe_2$ and WSe_2 remain less explored. However, studies show that selenide counterparts may be superior to sulfides in many aspects. Here we report a chemical vapor deposition growth of high-quality monolayer $MoSe_2$ and WSe_2 on sapphire substrate using metal oxides and solid selenium as precursors. Further investigation of the materials using optical and atomic force microscopies, as well as X-ray photoelectron, photoluminescence and Raman spectroscopies showed a high quality of the grown material.

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Ultrafast memristive switching utilising hidden collectively ordered many-body quantum states in 1T-TaS_2

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Many-body correlated electron states in metal TMDs are of fundamental interest beyond materials science. Hidden (false vacuum) states are distinct metastable states of matter which cannot be reached under non-equilibrium or non-ergodic conditions. Quasi-two-dimensional electronically ordered chalcogenide crystals systems, such as 1T-TaS_2 are particularly interesting from this point of view, because they exhibit competing orders already under equilibrium conditions. Here we show controllable ultrafast memristive switching between different macroscopically charge ordered states under highly non-equilibrium conditions initiated by either ultrashort laser[1] or electronic[2] excitation pulses. The switching mechanism attributed to a transient particle-hole imbalance which creates conditions under which a long-range ordered state can form. The hidden state is topologically distinct from the ground state, which accounts for unusually long lifetimes and leads to interesting applications[3]. I will show different ways to manipulate the hidden state transition experimentally, including detailed investigations on the stabilization mechanisms[4]. The large resistance change, record-breaking electrical (30 ps) and optical (35 fs) switching speeds, and ultralow energy per bit opens the way to new concepts in non-volatile memory devices manipulating all-electronic states in two-dimensional charge-ordered chalcogenide systems. Experiments on practical device performance will be presented and discussed.

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Peculiar piezoelectric properties of two-dimensional materials

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Recently, two-dimensional materials with non-centrosymmetric structure have received significant interest due to their potential usage in piezoelectric applications. In order to deeply investigate this potential, we performed first-principles calculations and systematically investigated the piezoelectric properties of various single layer structures, including transition metal dichalcogenide/oxides (TMDCs/TMDOs) monolayers and group II-VI compounds[2]. We found that the piezoelectric strain (d_{11}) and stress (e_{11}) coefficients of some of TMDCs are comparable or even better than that of conventional bulk piezoelectric materials. We predicted that not only the Mo- and W-based TMDCs but also the other materials with Cr, Ti, Zr, and Sn exhibit highly promising piezoelectric properties. By the help of alloying, we showed that the piezoelectric properties of MoS_2 monolayer can be significantly enhanced[2]. While alloying with W reduces the e_{11} and d_{11} coefficients, doping with Cr, S,e and Te atoms is an appealing way to improve piezoelectric properties of MoS_2. Moreover, we surprisingly observed that the calculated d_{11} coefficients of some of II–VI compounds are quite larger than that of TMDCs and the bulk materials, α-quartz, w-GaN, and w-AlN, which are widely used, in current applications[3]. Our calculations clearly reveal that monolayer semiconductors are strong candidates for future atomically thin piezoelectric applications such as transducers, sensors, and energy harvesting devices.

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Tuning the properties of two-dimensional materials by doping and heterostacking

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This talk will discuss the synthesis of large-area, high-quality monolayers of nitrogen-, boron- and silicon-doped graphene sheets on Cu foils using ambient-pressure chemical vapor deposition (AP-CVD). Scanning tunneling microscopy (STM) and spectroscopy (STS) reveal that the defects in the doped graphene samples arrange in different geometrical configurations exhibiting different electronic and magnetic properties. Interestingly, these doped layers could be used as efficient molecular sensors and electronic devices. In addition, the synthesis of hybrid carbon materials consisting of sandwich layers of graphene layers and carbon nanotubes by a self-assembly route will be discussed. These films are energetically stable and could well find important applications as field emission sources, catalytic supports, gas adsorption materials and super capacitors. Beyond graphene, the synthesis of other two-dimensional materials will be described. In particular, we will discuss the synthesis of WS_2 and MoS_2 triangular monolayers, as well as large area films using a high temperature sulfurization of WO_x clusters deposited on insulating substrates. We will show that depending on the substrate and the sizes of the oxide clusters, various morphologies of layered dichalcogenides could be obtained. In addition, photocurrent measurements on these materials will be presented. Our results indicate that the electrical response strongly depends on the laser photon energy. The excellent response observed to detect different photon wavelengths in MoS_2, WS_2 and WSe_2 materials, suggest these materials could be used in the fabrication of novel ultrafast photo sensors. We will also show that these techniques are able to produce in-plane heterojunctions with sharp interfaces of MoS_2 and WS_2. The material exhibits novel excitonic effects that will be discussed. Furthermore, a novel bottom-up method to create in-plane and vertical heterostructures of WS_2 and WSe_2 has been developed. The synthetic method involves the precursors tungsten hexacarbonyl ($W(CO)_6$) and hydrogen sulfide (H_2S) and hydrogen selenide (H_2Se). Selective growth was achieved on SiO_2 and sapphire and h-BN. Extensive characterization by Raman spectroscopy, atomic force microscopy, scanning and transmission electron microscopies revealed polycrystalline nature of these films, which can be grown as thin as a monolayer. This method enabled the fabrication of field effect phototransistors revealing mobility values comparable to those observed on CVD grown and exfoliated samples.

Electrochemical nature of ionic liquid gated Bi_2Te_3 transistors

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We have studied the intrinsic nature of double layer charging phenomenon in ionic liquid gated transistors based on various materials including a few-layer thick topological insulator, bismuth telluride (Bi_2Te_3) and distinguished between electrostatic and electrochemical regimes. Our work provides a guideline to understand the solid-liquid interfaces for a variety of materials and exclude the effect of pseudocapacitance that overestimates characteristic parameters of various materials. It focuses on applying electrochemical ionic liquid gating to Bi_2Te_3 and other materials to study interfacial electrochemistry. Ultrahigh electric fields (~30 MV/cm) are sustained by inducing large surface charge densities which have been measured by electrochemical impedance spectroscopy at room and higher temperatures, up to 400 K. Moreover, transport measurements above room temperature are reported and clarify high temperature solid-liquid interfacial electrochemistry.

Multilayer TMDC synthesis and phase conversion

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Transition metal dichalcogenides (TMDs) are van-der-Waals crystals and have attracted huge interest from the research community in the past five years. They have been used to promise high-performance ultra-thin electronics and photonics. Current TMD synthesis routes (CVD[1], MOCVD[2], ALD[3]), which are scalable, generally require high temperature and high cost equipment. Thermally assisted conversion (TAC) is reviewed as a synthesis method that addresses the issues of high-temperature and high-overhead in TMD synthesis.

An additional aspect that has had limited attention is the existence of several polytypes for many of the layered TMDs. Generally, these polytypes are not all isolatable during CVD and must be accessed by another route. Previously, organolithium chemistry has been applied to TMD particle suspensions[4] and partial monolayer films[5]. In this talk we report on the reaction of large scale TAC TMD films with organolithium chemistry.

MoS_2 and $MoSe_2$ films were treated with n-BuLi yielding a co-phase system of the 2H and 1T phase. The co-existence of the two phases was confirmed by spectroscopic and microsocpic methods. This is the first time polytype conversion has been applied to a continuous TMDC film with excellent prospects for phase-engineered devices.

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Static and dynamic optical properties of monolayer black phosphorus

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Black phosphorus is currently inciting a rapidly increasing scientific interest, due to the combined effect of a direct bandgap and of relatively high carrier mobilities, resulting in an on-off ratio for field effect transistors in excess of 10^5[1]. Many of its fundamental electronic and optical properties are still unclear, owing to its instability under atmospheric conditions. Here we present the results of the optical investigation of monolayer black phosphorus in terms of both static excitonic response[2] and exciton dynamics[3]. The samples were obtained by mechanical exfoliation in an Ar atmosphere. The monolayer character was confirmed by in-situ Raman spectroscopy on the same sample investigated by micro-photoluminescence (μPL) spectroscopy.

In Fig. 1(a) we show normalized low temperature (T = 4 K) μPL spectra measured at different excitation powers. The spectra are dominated by an intense emission line centered at ~2 eV and attributed to the recombination of the neutral exciton. A weaker peak is systematically observed at 1.84 eV and attributed to the recombination of the charged exciton[2]. In Fig. 1(b) we show temperature dependent μPL spectra of monolayer black phosphorus. The observed blue-shift of the emission is successfully explained by employing a two-oscillator model for the band gap[2]. The dependence of the dynamics of the neutral exciton recombination as a function of the excitation power is summarized in Fig. 1(c)[3]. At low excitation power, the temporal decay of the μPL can be successfully modeled with a double-exponential decay, with the shorter decay time related to the defect-mediated trapping and the longer decay time signature of the radiative recombination of the exciton. As the exciton population increases with an increasing excitation power, a fast, non-exponential decay component develops (see Fig. 1(c), bottom panel). In this condition, the observed temporal dependence is best described by a bimolecular model involving exciton-exciton annihilation.

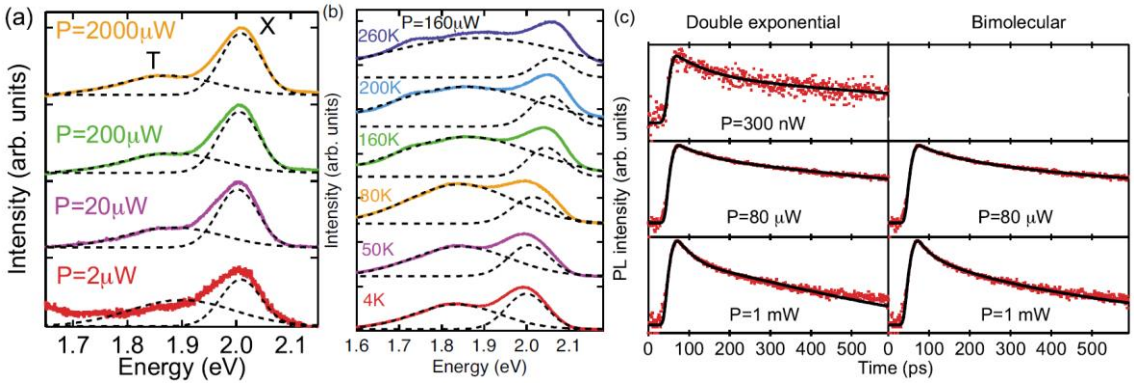

Figure 1 (a) Power dependent μPL spectra of monolayer black phosphorus. (b) Temperature dependence of the μPL of monolayer black phosphorus. (c) Power-dependent, time-resolved μPL (T = 4 K).

[1] Ling *et al.*, *Proc. of the Nat. Acad. of Sci. of USA* **112**, 4523 (2015).
[2] Surrente *et al.*, *Physical Review B*, in press (2016).
[3] Surrente *et al.*, in preparation.

Fermi polaron-polaritons in $MoSe_2$

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The truly 2D nature of transition metal dichalcogenides (TMDs) as well as their large electron mass infer strong Coulomb interactions which imply strong exciton binding energies of order 500 meV. The resulting small Bohr radius ensures a strong coupling of the exciton to light. Using a fiber microcavity, we measure cavity spectroscopy of gate-tunable monolayer $MoSe_2$ in the weak as well as in the strong coupling regime. In the weak coupling regime, we observe two resonances whose relative intensities change with the electron density. We find that both resonances show a sizable normal mode splitting which rules out their usual identification as exciton and trion but demonstrates that the elementary optical excitations in this new material system are attractive and repulsive polarons. Our findings completely revamp the current paradigm used to describe the ever-growing number of experiments based on TMD monolayers.

Label-free optical biosensor platform based on 2D inorganic semiconductors

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Two-dimensional (2D) material based on graphene and semiconductor transition metal dichalcogenides (TMDs) due to their superior electrical characteristics have been used as transducers in recent years for various sensor applications. In addition, novel optical properties exhibited by 2D semiconductors such as molybdenum disulphide (MoS_2) may provide the opportunities towards pushing the sensitivity limitations on current optical sensing methods which are widely used in molecular detection and especially in *in-vitro* diagnostics applications. Here we take MoS_2 as a candidate material to realize label-free optical sensing platform for the detection of non-labelled DNA molecules with high sensitivity. High quality MoS_2 flakes are chemically exfoliated from bulk and used as a source for the preparation of thin-films over glass substrates. These MoS_2-based thin-films display excellent fluorescence characteristics and are employed for realizing a Förster resonance energy transfer (FRET) based molecular detection mechanism. Labelled receptor DNA molecules are functionalized on the MoS_2 films using a brand-new functionalization technique where onset of FRET pair between MoS_2 and 'dye' is accentuated or diminished in the presence of complementary analyte DNA molecules. In this way, we were able to realize an on-chip sensor platform for the detect DNA concentrations as low as few nanomolar in a label-free method using a fluorescence microarray scanner. Label-free optical assays with such optical platforms may provide versatile solutions in diagnostics industry and overcome current limitations associated with labelled optical detection techniques.

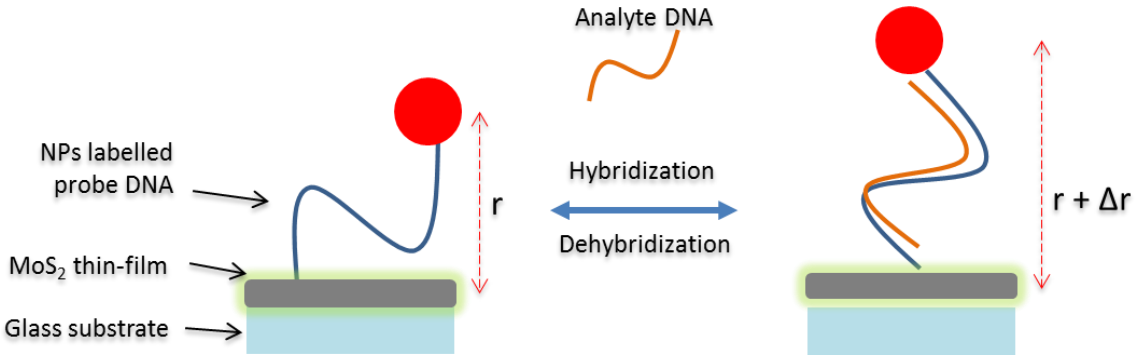

Figure 1 FRET based label-free optical sensing of DNA on MoS_2 thin-films.

[1] V Pachauri, K Kern, K Balasubramanian, "Chemically exfoliated large-area two-dimensional flakes of molybdenum disulfide for device applications", *APL Materials* 2013, **1** (3), 032102.

Frustration and order in insulating and superconducting monolayers of $(BETS)_2GaCl_4$ on Ag(111)

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The capability to fabricate crystalline monolayers of confined superconducting or magnetic condensate on surfaces is essential to realize new functionalities and understand the nature of competing orders in their phase diagram at the nanoscale. Herein, we outline a reliable method to pattern a monolayer of superconducting islands and Kagome lattice of $(BETS)_2GaCl_4$ (where BETS = bis(ethylenedithio) tetraselenafulvalene) on Ag(111). At a deposition temperature of 125 K, $(BETS)_2GaCl_4$ dimers form Kagome lattice with a pore size of 1.2 nm, making it possible to encapsulate small molecules within the nanoporous network. When deposited at 300 K, the molecules retain their superconducting structure and minimize substrate interaction by aligning their long molecular axis perpendicular to the substrate. These results provide guidelines for facile controllable fabrications of epitaxial superconducting and/or magnetic confined condensates on metal surfaces. Finally, we will describe our attempt to map the proximity effects near the edges of the islands.

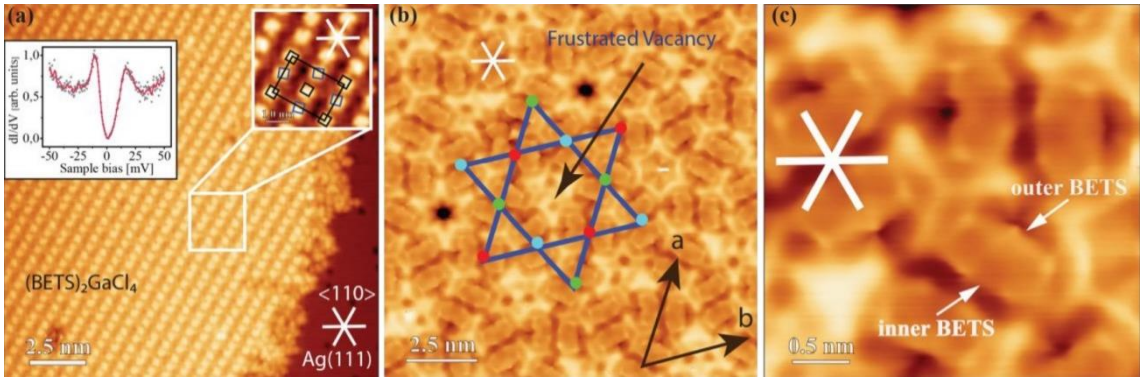

Figure 1 Single layer of $(BETS)_2GaCl_4$ superconductor and Kagome lattice on Ag(111).

[1] A. Hassanien *et al.*, "Epitaxial growth of insulating and superconducting monolayers of $(BETS)_2GaCl_4$ on Ag(111)", *physica status solidi* **252**, 11, 2574 (2015).
[2] K. Clark *et al.*, "Superconductivity in just four pairs of $(BETS)_2GaCl_4$ molecules", *Nat. Nanotechnol.* **5**, 261 (2010).

1 Raman modes in layered $(M(X))_n(TX_2)_m$ heterostructures (M – metal, T – transition metal, X – chalcogen)

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Layered heterostructures consisting of alternating layers of metal chalcogenides (MX) and transition-metal dichalcogenides (TX_2) have been studied for decades now. They can be synthesized either in bulk (3d)[1], or (more recently) nanotube (1d)[2] phase. In the Raman spectra of these compounds, peaks of the zone-centered phonon modes originating from the guest (MX) layers can be clearly distinguished from the ones originating from the host (TX_2) layers. This is expected, since the layers are assumed to interact predominantly by weak van der Waals forces. Moreover, one would expect that the frequencies of such "hetero-structured" modes be only slightly different from the frequencies of the corresponding "homo-structured" modes. However, this is not always the case: E_g modes of the host TX_2 layers in the heterostructure can experience significant frequency shifts (up to 40 cm^{-1} !) with respect to the corresponding pure TX_2, while the A_g modes remain almost unshifted[3]. In attempt to explain this unusual behaviour, we perform first-principle density functional theory (DFT) and density functional perturbation theory (DFPT) calculations on selected heterostructures. The results are compared to available experimental data, and used to gain a deeper insight into the nature of inter-layer bonding of layered heterostructures.

[1] Wiegers, G. A., Meetsma, A. & de Boer, J. L. "Crystal growth, structure and some properties of $PbNbS_3$, $SnSNbS_3$, $LaNbS_3$ and related misfit layer compounds", *Solid State Ionics* **33,** 183–191 (1989).

[2] Radovsky, G., Popovitz-Biro, R., Stroppa, D. G., Houben, L. & Tenne, R. "Nanotubes from Chalcogenide Misfit Compounds: Sn-S and Nb-Pb-S", *Acc. Chem. Res.* **47,** 406–416 (2014).

[3] Hangyo, M., Nakashima, S., Hamada, Y., Nishio, T. & Ohno, Y. "Raman scattering from the misfit-layer compounds $SnNbS_3$, $PbNbS_3$, and $PbTiS_3$", *Phys. Rev. B* **48,** 291–297 (1993).

2 Optical fingerprint of dark 2p-states in transition metal dichalcogenides

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We present a microscopic study on higher excitonic states in transition metal dichalcogenides in the presence of disorder. In agreement with recent studies, we show that the geometric phase cancels the degeneration of 2s and 2p states. Our results reveal a significant disorder-induced coupling of bright s and dark p states offering a strategy to circumvent optical selection rules in these materials. As a proof, we show a direct fingerprint of 2p states in linear absorption spectra of WS_2. The predicted softening of strict optical selection rules through exciton-disorder coupling is of general nature and therefore applicable to related two-dimensional semiconductors.

3 Atomically thin $MoSe_2$ nanostructures grown by molecular beam epitaxy

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Transition metal dichalcogenides (TMDs) together with other two-dimensional (2D) materials have attracted great interest due to the unique optical and electrical properties of atomically thin layers. In order to fulfill the potential roadmaps, developing the large-area growth of transition metal dichalcogenides has become crucial. Here, we used molecular beam epitaxy (MBE) to grow atomically thin $MoSe_2$ on GaAs(111), and the growth was *in-situ* monitored by reflection high-energy electron diffraction (RHEED). Photoluminescence (PL) of nominal monolayer (ML) $MoSe_2$ at room temperature showed a peak of 1.58 eV. The first few layers were formed *via* van der Waals epitaxy with no detectable strain, and no intermediate compounds were found at the interface in X-ray photoluminescence spectra (XPS).

The nanostructures under scanning transmission electron microscopy (STEM) exhibited two misoriented domains with ~15° difference and result in prevailing misoriented bilayer (BL) regions over 70%. A nucleation mechanism is proposed to explain the overgrowth, implying that the edges may be preferential nucleation sites. The results demonstrate the potentials of MBE technique for large-area growth and also reveal fundamental features of van der Waals epitaxy.

4 Thiol click chemistry on gold-decorated MoS_2: elastomer composites and structural phase transitions

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Research on layered semiconducting transition metal dichalcogenides (TMDs) is growing rapidly, driven by the possibility to improve devices in different areas of research from electronics, photonics to chemical catalysts.

Chemical exfoliation using *n*-butyllithium (*n*-butyl:Li) allows the exfoliation of comparatively large amounts of material and stands out from the other methods in that it largely transforms semiconducting TMDs from their stable 2H into the metallic 1T phase. This metastable phase can be transformed back to 2H through heating. We have developed a procedure for decorating chemicaly exfoliated MoS_2 flakes with gold nanoparticles (GNP). TEM images confirm the crystal structure of gold and show that the GNPs, with typical diameters around 2 nm only slightly coalesce upon thermal treatment at up to 400 °C.

Thiol chemistry drives progress in areas ranging from molecular electronics to biosensors. In particular, thiol-ene click chemistry enables tunable polysiloxane-based elastomers, such as poly[(mercaptopropyl)methylsiloxane] (PMMS), whose cross-linking can be activated photochemically or thermally. A thiol group at each repeat unit along the backbone allows for strong cross-linking, while the high molecular weight (ca. 4–7 kg/mol) eliminates the traditional odor problems of thiols.

Subsequently, we have found that PMMS enables to disperse both metallic and semiconducting flakes in the same solvent, and used optical absorption and Raman spectroscopy to show transformation from the metallic to the semiconducting phase without restacking both in dispersion and as fillers of an elastomer nanocomposite. Finally, by using different flakes (decorated and undecorated, different defect content) and PMMS with different degrees of thiolation, we identified the interaction between the thiol groups and the GNPs as the driving force for the nanocomposite formation.

[1] P. Topolovsek *et al.*, "Thiol click chemistry on gold-decorated MoS_2: elastomer composites and structural phase transitions", *Nanoscale* **8** (2016): 10016–10020.

5 Comparison of radiative and Auger recombination of free trions in tungsten based 2D transition metal dichalcogenides

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Monolayer transition metal dichalcogenides (TMDCs) possess unique properties[1], making them promising for creating nm-thin optoelectronic devices[2]. However, non-radiative processes can limit the efficiency of these materials in optoelectronics applications. Tungsten based TMDCs (WX_2, X = S, Se), as opposed to their molybdenum counterparts, have a reversed spin splitting ordering in the conduction and valence bands, resulting in a semi-dark trion ground state (Fig. 1), where radiative recombination is prevented by spin and momentum conservation. However, the trion can get excited to a state where the electrons and hole reside in the same valley and can recombine radiatively. As a result, the photoluminescence spectrum is expected to contain a line shifted from the ground state trion energy by the conduction band spin splitting and having an activation behaviour determined by the size of the conduction band spin splitting. In the bright trion state, a novel Auger-type process made possible by the unique band structure of TMDCs[3] and assisted by phonon emission can compete with the radiative process (Fig. 2). We calculate the non-radiative transition rate, finding an increasing rate with increasing temperature, and compare to the rate of the radiative process. We find that the radiative process is more efficient at low temperatures, however at room temperature, the two rates can become comparable and the radiative process can be supressed.

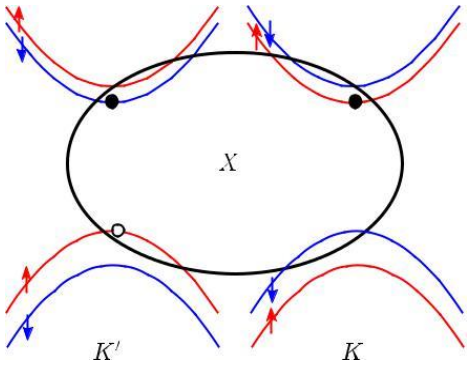

Figure 1 Sketch of the WX_2 band structure and spin splitting at the K/K' points of the Brillouin zone, and the ground state trion consisting of electrons in separate valleys and a hole.

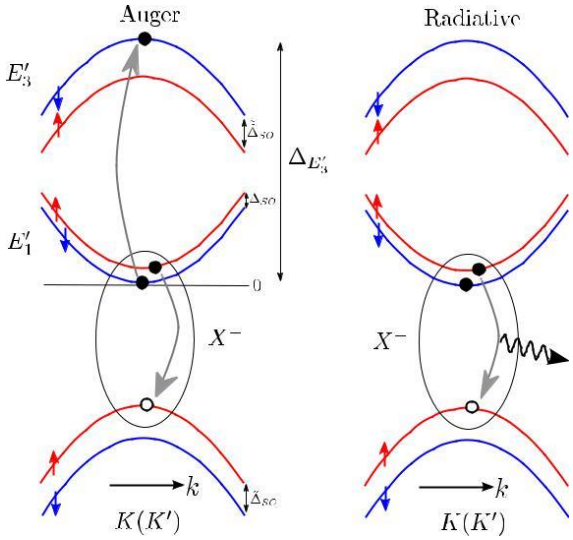

Figure 2 Sketch of the Auger (left) and radiative (right) recombination processes in WX_2.

[1] Qing Hua Wang, Kourosh Kalantar-Zadeh, Andras Kis, Jonathan N. Coleman, Michael S. Strano, Nature *Nanotechnology* **11**, (2012), 699.

[2] Deep Jariwala, Vinod K. Sangwan, Lincoln J. Lauhon, Tobin J. Marks, Mark C. Hersam, *ACS Nano* **2**, (2014), 1102.

[3] Andor Kormnyos, Guido Burkard, Martin Gmitra, Jaroslav Fabian, Viktor Zolyomi, Neil D. Drummond, Vladimir Fal'ko, *2D Materials* **2**, (2015), 022001.

6 Perovskite-type oxide nanosheets doped with magnetic elements: synthesis and structure

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We have reported that a series of 2D oxide nanosheets with a progressively controlled thickness were derived from a homologous family of layered perovskite niobates, $KNa_{n-3}Ca_2Nb_nO_{3n+1}$ ($n = 3-6$), through soft-chemical delamination processes[1]. In this work, synthesis of a new homologous compounds doped with magnetic elements, e. g Mn, Fe, Co and Ni, was attempted by applying the "solid-state templating method". Resulting phases were exfoliated into new perovskite-type nanosheets.

A stoichiometric mixture of the layered perovskite, $ACa_2Nb_3O_{10}$ (A = K or Rb), and ilmenite-type oxide, $MTiO_3$ (M = Mn, Fe, Co and Ni), was heated at 1373 K to synthesize target compounds. The XRD data and chemical analysis indicate the successful formation of the $n = 4$ member, $ACa_2MNb_3TiO_{13}$. The obtained samples were converted into H^+-exchange forms, $HCa_2MnNb_3TiO_{13}$ upon treatment with a HNO_3 solution, which were further reacted with an aqueous solution containing tetrabutylammonium ions. A turbid colloidal suspension was obtained through this process. AFM observation of the dispersed sample after depositing on a Si substrate detected micrometer-sized 2D objects with a uniform thickness of ~2.1 nm (Figure 1), suggesting the delamination into unilamellar nanosheets. In-plane and out-of-plane XRD data further support the full exfoliation of the layered perovskite compounds.

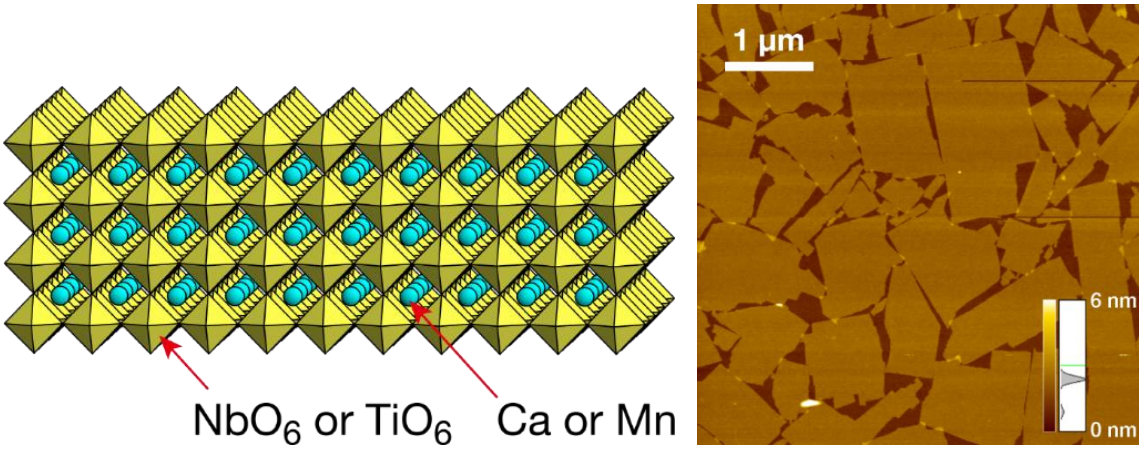

Figure 1 Schematic structure and AFM image of $Ca_2MnNb_3TiO_{13}$ nanosheets.

[1] Y. Ebina, K. Akatsuka, K. Fukuda, and T. Sasaki, "Synthesis and In Situ X-ray Diffraction Characterization of Two-Dimensional Perovskite-Type Oxide Colloids with a Controlled Molecular Thickness", *Chem. Mater.* **24** (2012), 4201.

7 Effect of discrete breathers in the thermal conductivity of graphene: a molecular dynamics study

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Intrinsic localized modes or discrete breathers (DB) are investigated by molecular dynamics (MD) simulations in free-standing graphene. Discrete breathers are generated either through thermal quenching of the graphene lattice or by proper initialization. In a realistic scenario, *i. e.* temperature-dependent MD simulations in three dimensions using a graphene-specific interatomic potential[1], the DBs lifetimes are about hundreds of picoseconds even at high temperatures ($T > 1500$ K). These long lifetimes may enable direct DB observation in Raman spectroscopy experiments[2]. Recently, the thermoelectric properties of graphene and graphene structures have attracted significant attention from the physics and engineering communities[3–5]. In this work the effect of these DBs in thermal transport is being investigated. Possible ways to tune the thermal conductivity in graphene are examined.

[1] L. Lindsay and D. A. Broido, "Optimized Tersoff and Brenner empirical potential parameters for lattice dynamics and phonon thermal transport in carbon nanotubes and graphene", *Phys Rev B* **81**, 205441 (2010).

[2] A. Fraile, E. N. Koukaras, K. Papagelis, N. Lazarides and G. P. Tsironis, "Long-lived discrete breathers in free-standing graphene", *Chaos, Solitons and Fractals* (In press).

[3] P. Dollfus, V. H. Nguyen and J. Saint-Martin, "Thermoelectric effects in graphene nanostructures", *J. Phys.: Condens. Matter* **27** (2015) 133204.

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8 Point contacts in encapsulated graphene

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Hexagonal boron nitride (hBN) encapsulated graphene can show outstanding electrical performance[1]. So far the best electrical contacts to these heterostructures were achieved by metallizing the edge of the graphene sheet (1D contacts)[2]. We demonstrate a novel contacting technique to create point contacts in the middle of the graphene sheet by using a top-hBN flake with drilled holes prior to dry-stacking assembly[3]. 2- and 4-terminal field effect measurements between a couple of point contacts of the same graphene sheet were performed and the results are in qualitative agreement with an electrostatic model assuming point-like contacts. In addition, in sufficiently large perpendicular magnetic field these field effect measurements show insulating behaviour corresponding to the quantum Hall effect in case of point contacts. The diameter of the point contacts was about 100 nm and the holes were obtained by focused ion beam drilling. This method can place inner contacts to a graphene sheet and is compatible with high mobility graphene samples at the same time, thus offering a large variety of further applications, *e. g.* in electron optics experiments.

[1] D. C. R., Y. A. F., M. I., L. C., W. L., S. S., W. K., T. T., K. P., S. K. L., and H. J., "Boron nitride substrates for high-quality graphene electronics", *Nature Nanotechnology*, vol. **5**, pp. 722726, Oct. 2010.

[2] L. Wang, I. Meric, P. Y. Huang, Q. Gao, Y. Gao, H. Tran, T. Taniguchi, K. Watanabe, L. M. Campos, D. A. Muller, J. Guo, P. Kim, J. Hone, K. L. Shepard, and C. R. Dean, "One-dimensional electrical contact to a two-dimensional material", *Science*, vol. **342**, no. 6158, pp. 614617, 2013.

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9 Dominant excitonic transitions in transition metal dichalcogenides

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Novel two-dimensional materials from the group of layered transition metal dichalcogenides (TMD) have recently attracted scientific interest for their unusual physical properties.

An interesting quality is their strong optical response that stems from the quantum confinement of electrons and holes in the quasi-2D geometry. The modified screening strongly enhances the binding of electron-hole pairs leading to binding energies of the lowest-lying excitonic transition of magnitude 0.5 eV in Mo and W based TMDs[1–4]. Despite this, a closer analysis of the nature of the excitonic transitions contributing to observed absorption peaks is still lacking so far.

We have thus performed *ab initio* calculations of the theoretical absorption spectra including electron-hole interaction for a range of mono- and bilayer transition metal dichalcogenides in trigonal-prismatic and octahedral phases and analyzed the *k*-space representation and spatial extent of the dominant excitons for excitation energies up to 3 eV. Our results suggest that changes of the electronic structure from variation of the chalcogen atoms and interlayer interactions lead to a noticeable qualitative evolution of the dominant transitions and can be explained by band nesting between valence and conduction bands.

[1] Qiu *et al.*, *Phys. Rev. Lett.* **111**, 216805 (2013).
[2] Umeda *et al.*, *Nature Materials* **13**, 1091 (2014).
[3] Yang *et al.*, *ACS Nano* **9**, 6603 (2015).
[4] Hanbicki *et al.*, *Sol. Stat. Comm.* **203**, 16 (2015).

10 Zirconium disulfide nanodiscs

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[b]*Yonsei-IBS Institute, Yonsei University, Seoul, Korea*
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We present a colloidal synthesis of ultrathin ZrS_2 (UT-ZrS_2) nanodiscs that are *ca.*1.6 nm thick. The lateral size of the discs can be tuned to 20, 35, or 60 nm while their thickness is fixed. Under the appropriate conditions, these individual discs can be self-assembled into face-to-face-stacked structures containing multiple discs. Because the S–Zr–S layers within individual discs are held together by weak van der Waals interactions, each UT-ZrS_2 disc provides spaces that can serve as host sites for intercalation. When we tested UT-ZrS_2 discs as anodic materials for Li^+ intercalation, they showed excellent nanoscale size effects, enhancing the discharge capacity by 230% and greatly improving the stability in comparison with bulk ZrS_2. The nanoscale thickness and lateral size of UT-ZrS_2 discs are critical for fast and reliable intercalation cycling because those dimensions both increase the surface area and provide open edges that enhance the diffusion kinetics for guest molecules.

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11 Electrostatic design in action: modifying electronic properties of molybdenum disulphide using adsorbed organic molecule

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In recent years there has been an increased interest in 2D materials because of their unique properties. Molybdenum disulphide (MoS_2) is one such 2D material that exhibits thickness-dependent electronic properties and is in the focus of contemporary research. Building upon the idea of using collective electrostatic effects for tuning the electronic structure of graphene[1], here we extend this strategy to pristine and doped molybdenum disulphide. By means of dispersion-corrected density functional theory simulations we find that compared to graphene, MoS_2 is more viable for electrostatic design as the shift in electrostatic potential due to adsorption of polar molecule is significantly larger than what has been predicted for graphene. For doped MoS_2 layer we furthermore investigate to what degree electrostatically patterning the MoS_2 surface can be useful for spatially localizing the doping-induced excess charges. Finally, we outline strategies for using (structurally) more complex molecules on MoS_2 for achieving complicated patterns in the electronic landscape such as valleys and islands.

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12 Synthetic strategy for single-layer transition-metal chalcogenides

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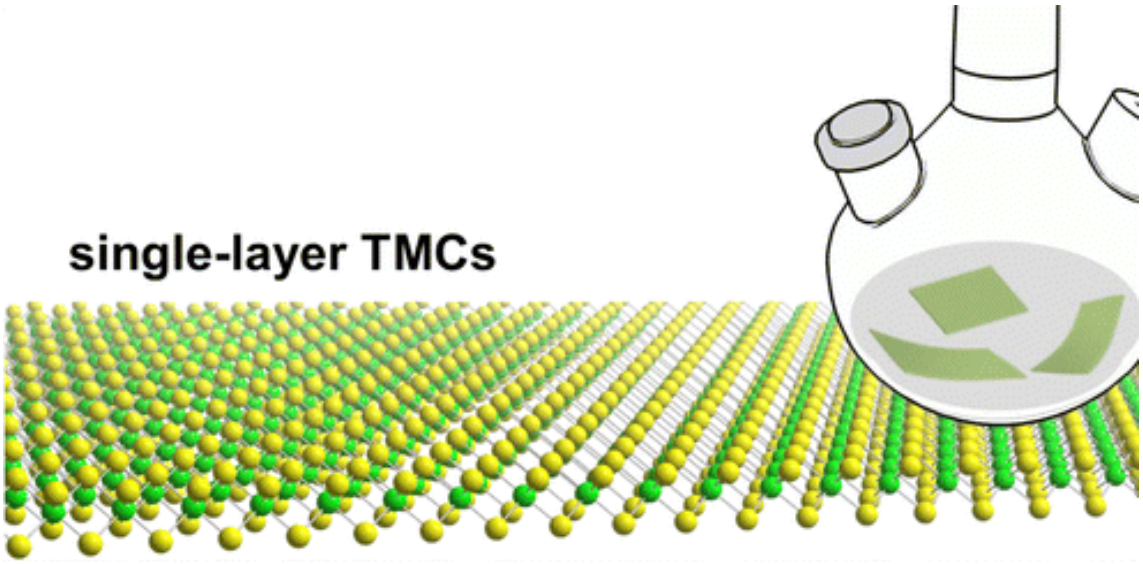
Two-dimensional (2D) single-layer transition-metal chalcogenides (TMCs) are considered as next generation 2D materials beyond graphene especially for applications such as optoelectronics, photocatalysis, and solar energy harvesting[1]. However, current solution-phase synthetic protocols have not been suitable for single-layer 2D TMCs due to the spontaneous formation of multilayer sheets.

We discovered a solution-phase synthetic protocol, called "diluted chalcogen continuous influx (DCCI)", where continuous influx of dilute H_2S throughout the entire growth period provides large sheet formation through the exclusive *a*- and *b*-axial growth processes[2]. Our DCCI protocol is a new synthetic concept for single-layer TMCs and, in principle, can be operative for wide range of TMC nanosheets.



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13 Raman spectroscopy and photoluminescence of misfit layer compound nanotubes from CrS_2

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Misfit layer compounds (MLC) offer an interesting approach towards synthesis of novel one-dimensional nanostructures and two-dimensional materials. Understanding their structure and their physical properties has been subject to intense scientific research. The MLCs described by the formula RX-TX_2 consist of a transition metal dichalcogenide (TMD) layer TX_2 and an intercalation layer RX with distorted rocksalt structure. Here R denotes one of the rare earth metals, X is one of the elements S or Se and T is an element of the group of transition metals.

In our study the TMD layer CrS_2 is intercalated by either a LaS-, CeS- or GdS-layer. Upon formation of the MLC, charge transfer between the sublayers and deformation of the intercalation layer stabilize the otherwise metastable CrS_2[1]. Due to the misfit between the sublayer in at least one direction and the seaming of dangling bonds at the rim atoms, the synthesis of nanotubes and scrolls is favoured[2]. We investigate the vibrational properties of MLC nanotubes *via* Raman spectroscopy and the optical properties *via* photoluminescence. The results are discussed regarding previous work on synthesis and TEM measurements of the MLC nanotubes[1–3].

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14 Solution processed electronics from 2D materials

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The liquid phase exfoliation (LPE) of 2D materials has meant their exotic properties can be incorporated into device manufacture using established deposition techniques. Processes such as inkjet printing and spray-coating can provide the dimensional definition required for some devices but in order to fully take advantage of these techniques, a comprehensive development of the deposition methods in concert with the establishment of a family of functional inks is critical for the production process.

A printed film composed purely of 2D materials is a porous nanoflake network (PNN) and hence is prone to containing pores large enough to expose the substrate layer. This is a fundamental challenge for vertically stacked films as these pores, or pinholes, will allow undesired contact between layers and will prevent the construction of heterostacks. Here, a process has been developed which incorporates inkjet printing of conductive graphene electrodes and spray-coating of a pinhole-free dielectric boron nitride layer with thicknesses ranging from 1.65 to 5.15 μm. The devices displayed capacitances ranging from 2.36 pF to 10.1 pF indicating successful creation of pinhole-free films.

The family of TMDs has provided the means to offset the lack of an intrinsic band gap in graphene. Here, we also describe a method for using the spray-coating technique to create graphene and WSe_2 films that can be gated using an ionic liquid. The use of a liquid gate means the porosity of the films can be exploited to maximise electrical output.

To demonstrate the simplicity and compatibility of the printing technique, we have created highly conductive lines from silver nanoplatelets using a desktop printer. The jetting parameters are fixed in these machines and thus a facile ink production method will show the strength of this deposition technique.

15 Long-lived circular polarization of defect photoluminescence of liquid exfoliated tungsten disulphide

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Monolayer transition metal dichalcogenides (TMDs) are a family of materials in which the valley pseudospin can be selectively addressed through circular polarization of optical transitions[1]. This property makes TMDs exciting in view of applications in novel information processing schemes. However, before any devices are realized, detailed understanding of the intervalley scattering processes is needed. In this work we show that the valley lifetime can be enhanced, if the bright exciton recombination is switched off.

We investigate steady-state and time resolved photoluminescence (PL) polarization of tungsten disulphide (WS_2) nanosheets obtained *via* liquid exfoliation[2]. This versatile and inexpensive technique allows to obtain large quantities of monolayer TMDs and thus is perfect for applications. Studying the temperature dependence, the temporal stability, and splitting in magnetic field, we demonstrate that at 10 K the PL is dominated by localized excitons. Our results strongly suggest that the localization occurs on the edges of the WS_2 nanosheets. The presence of this PL channel switches off the recombination *via* free excitons. The PL exhibits a robust circular polarization induced by the circularly polarized excitation and inherited from the valley-polarized free excitons. Time-resolved studies reveal that the PL decays in about 10 ps – a process controlled by non-radiative recombination. The polarization exhibits two decays – a short one occurring on a timescale of 20 ps and a long one significantly exceeding the PL lifetime.

We interpret the observed polarization dynamics as resulting from an existence of a reservoir of valley polarized excitons. We propose that this reservoir is the dark exciton state, which is known to exhibit a suppressed inter-valley scattering and in tungsten dichalcogenides is the exciton ground state[3]. Thus, after photoexcitation, this dark state is preferentially populated leading to an enhancement in the valley lifetime reflected in the long-lived circular polarization of the PL signal. We employ a rate equation model accounting for the proposed relaxation pathway. The calculations qualitatively reproduce the measured PL and polarization dynamics.

Our results demonstrate the influence of the dark excitons and the presence of defects on the valley dynamics. Moreover, the results show that liquid exfoliation constitutes a viable alternative for other monolayer TMD fabrication methods in terms of studies of the valley effects and design of future valley devices.

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16 Piezoresistivity and strain-induced band gap tuning in atomically thin MoS_2

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Atomically thin membranes such as MoS_2, exhibit high Young's modulus and fracture strength[1] which makes them viable candidates for modifying their properties *via* strain[2]. The bandgap of MoS_2 is predicted to be highly strain-tunable[3] which results in a modulation of its electrical conductivity through the piezoresistive effect[4].

Here we incorporate monolayer, bilayer and trilayer MoS_2 in a nanoelectromechanical membrane configuration. Strain-induced bandgap tuning is detected *via* electrical conductivity measurements and the emergence of piezoresistive effect in MoS_2 is demonstrated. We observe a continuous and reversible bandgap modulation in atomically thin MoS_2 membranes with a thickness dependent modulation rate. Finite element method (FEM) simulations are used to obtain a comprehensive picture of the spatially varying bandgap profile on the membrane and to quantify the rate of bandgap change. The piezoresistive gauge factor is calculated for single layer, bilayer and trilayer MoS_2. Our results reveal that atomically thin MoS_2 membranes show strong piezoresistive effect which is comparable to the state-of-the-art silicon strain sensors[5] and two orders of magnitude higher than graphene strain sensors[6].

Controllable modulation of resistivity in 2D nanomaterials using strain-induced bandgap tuning offers a novel approach for implementing an important class of NEMS transducers, self-sensing resonators, strain sensors, flexible and wearable electronics, tunable photovoltaics and photodetection.

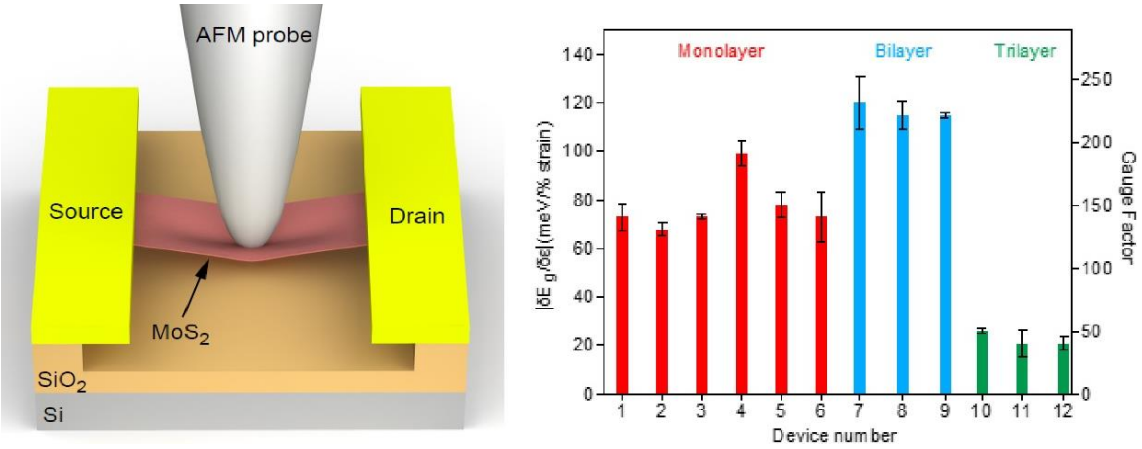

Figure 1 (a) Schematic drawings of setup. (b) Measured values of bandgap change rate and piezoresistive gauge factor for monolayer, bilayer and trilayer MoS_2.

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17 Sensing nanomasses with resonant acoustic modes of 2D colloidal nanoplatelets

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[b]*Laboratoire Interdisciplinaire Carnot de Bourgogne, CNRS-Université de Bourgogne, France*
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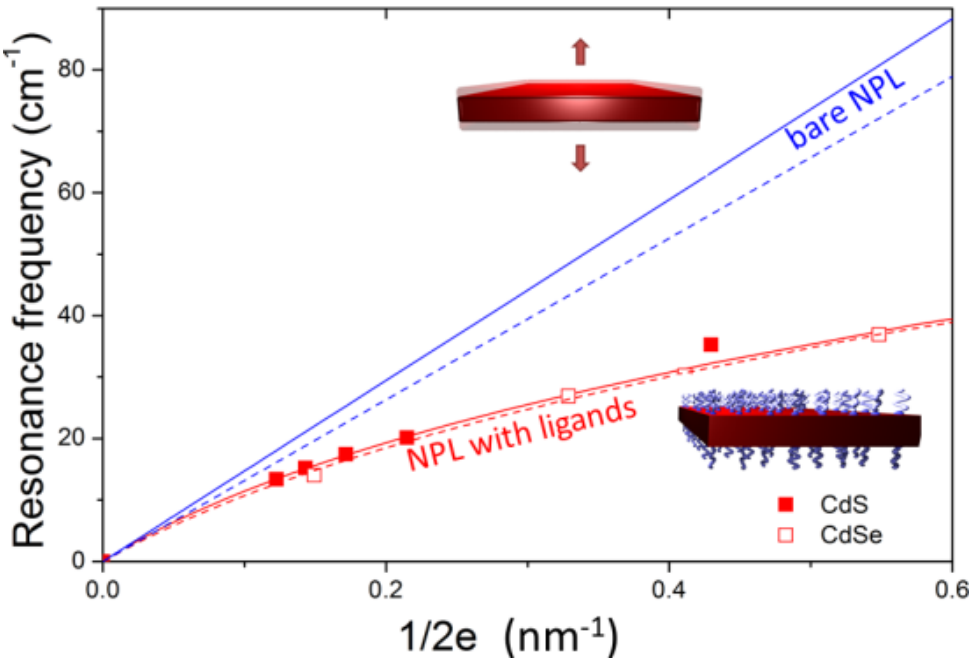
Resonant acoustic modes confined in semi-conductor nanoplatelets with nanometer thicknesses were studied using low frequency Raman scattering (LFRS). The frequencies of these modes depend on the elastic constants of the material, thereby providing an elastic characterization of the nano-objects. If LFRS has been widely used to characterize the elasticity of spherical nano-objects[1,2], applications to 2D nanoplates are scarcer. We show that probing low frequency Raman modes from large surface-to-volume ratio 2D nanoplatelets turns out to allow sensing of nanomasses.

The samples studied are CdS and CdSe nanoplatelets synthesized through the colloidal route, with thicknesses ranging between a few monolayers (~1 nm) and a dozen MLs (~4 nm). The analysis of the thickness breathing mode as a function of reciprocal thicknesses reveals significant deviations with respect to the expected behavior of plain plate geometries, as observed from exfoliated nanosheets[3]. We show that these deviations can be quantitatively described by the significant additional weight of surfactant molecules bound to the extended top and bottom faces of the platelets.



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18 Thermoelectric properties of 2D semiconductors

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We investigate the thermoelectric properties of thin layers of MoS_2 and $MoSe_2$. Microfabricated electrodes acting as thermometers and heater allow the simultaneous measurement of electronic and thermal effects. We use the 2ω technique to determine the thermoelectric power voltage induced due to a temperature gradient across the device achieved by heating the flake locally. The Seebeck coefficients determined by the measurements show a strong dependence on the doping of the 2D materials and can be higher than those of conventional thermoelectric materials. These results represent a basis for the future application of ultrathin 2D materials for thermoelectric power generation.

19 Transition metal dichalcogenide heterostack p-n junction diodes

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Transition metal dichalcogenide (TMD) 2D nanomaterials have shown great promise for a wide variety of applications in both electronics and optoelectronics. However, for these applications to be realised, large scale, reproducible and timely growth of these materials must be achieved. Thermally assisted conversion of pre-deposited metal films offers a pathway to grow these TMDs and fulfils many of the requirements of an industrial scalable process. This could provide a promising way forward from lab scale demonstration of principle for TMDs. There are a host of promising TMDs available, with the field of potential applications further expanded by combining different TMD films to create vertical and horizontal heterostacks.

Heterostack p-n junction diodes are created from a number of different TMDs using thermally assisted conversion[1]. The pre-deposited films are molybdenum, tungsten or platinum which are then converted in a CVD furnace in the presence of either sulphur or selenium. Various mean of creating heterostacks are examined such as co- and sequential conversion of the films, along with transfer stacking of already converted films. The TMD stacks are characterised using Raman spectroscopy, AFM, XPS and electron microscopies. Of particular interest is the interface between the two layers and how this changes depending on production method and temperature. Finally these properties are related to the optoelectronic properties of the heterostacks.

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20 Doping and alloying made simple: how to maximize the potential of transition metal dichalcogenides

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Transition metal dichalcogenides (TMDs) are trending as promising materials for a large verity of applications such as photocatalysis, photonics, photovoltaic devices, thin layer transistors, super capacitors and many others. Precise control over morphology and composition of the TMDs is crucial and should be tailored for each specific application. Traditional solid state techniques such as chemical vapour deposition (CVD) or chemical vapour transport (CVT), while simple and well established for producing flat, single or few layers TMDs, become inefficient when required to produce large scale, homogeneous constructs with complicated morphologies.

We have shown that colloidal synthesis can be used to produce TMD alloys as well as to dope TMDs with other atoms, thus obtaining control over their electronic and catalytic properties. Choosing to focus on photocatalysis, we produce thin edge nanoflowers of $Mo(S_xSe_{1-x})_2$ alloys as well as Fe-doped MoS_2 and $MoSe_2$ as model systems to show the versatility of the method. Various analytical methods were used to determine the formation mechanism, composition and structure of the products as well as their electrochemical and photocatalytic performance. We were able to determine that for this specific approach, the formation mechanism initiates from the precipitation of amorphous homogeneous substance. It then crystallizes into curled and tangled sheets of the appropriate TMD enabling the production of homogeneous alloys or doped constructs.

Electrochemical and hydrogen production measurements showed that Fe-doped MoS_2 and $MoSe_2$ have superior performance to pure MoS_2 and $MoSe_2$ when the Fe is homogeneously distributed in the nanoflower structure. By successfully modifying the electronic and catalytic properties of TMDs using colloidal synthesis we have opened the door for additional tuning and optimization of TMDs for other applications such as photonics, super capacitors or batteries.

21 Size and shape-controlled synthesis of semiconducting nanomaterials

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Semiconducting materials have many promising applications from optoelectronic devices to biological field. This large family of chemical compounds has a variety of optical, electronic and mechanical properties arising from their different composition and morphology. Moreover, smaller and more effective devices can be produced by decreasing the particles size to the nanoscale. In this regard, the design of suitable routes for the preparation of semiconducting nanomaterials still remains a challenge in the field.

There are different synthetic approaches to obtain semiconducting nanoparticles including wet-chemistry methods (solvothermal/hydrothermal and sol-gel techniques), which have shown great potential for the preparation of nanostructures with a controlled shape and size[1,2]. In this work, we explore the versatility of wet-chemistry to direct the growth of different layered semiconducting nanomaterials with a defined shape and size by the use of templating agents.

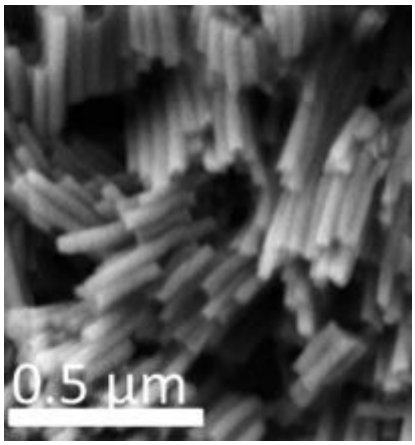

Figure 1 Scanning electron microscopy image of long-chain amine-templated gallium sulfide nanotubes.

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22 Exciton-phonon and electron-phonon coupling in MoS_2

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Two-dimensional layered 'van der Waals' materials are of increasing interest for fundamental research as well as device applications in the areas of electronics, spin- and valleytronics, as well as optoelectronics and sensing. Beyond graphene, the transition metal dichalcogenide (TMDC) family is subject of intense investigations for device applications due to their electronic band gap in the visible range, their stability and inertness in aqueous environment[1].

We utilize Raman spectroscopy on pristine MoS_2 flakes as well as on MoS_2 field-effect transistor (FET) devices to compare the effect of photo-doping with electrostatic doping in mono- and few-layer MoS_2[2]. In non-resonant Raman measurements, a strong power- and gate-voltage dependence of first order phonon modes is observable[2]. Resonant Raman spectroscopy reveals an unexpected polarization dependence of the first-order modes that is dependent on the charge carrier density and points towards the importance of exciton-phonon coupling in the resonant light scattering process[3].

Furthermore, a resonantly activated two-phonon scattering process involving longitudinal acoustic phonons (2LA) exhibits an electron density dependent redshift that can be interpreted as renormalization of the LA mode at the M-point. The LA mode at the M-point is assumed to mediate the superconductivity by connecting the Fermi seas at the nearly degenerate K- and Λ points[4].

Our findings demonstrate the importance of interaction of phonons with the electronic systems in 2D materials that can be greatly tuned by the charge carrier density.

We acknowledge fruitful discussion with Alexander Högele and Jessica Lindlau and financial support by the DFG excellence cluster 'Nanosystems Initiative Munich (NIM)'.

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23 Chemically derived thin-films of molybdenum disulphide and graphene oxide at wafer scale

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A new approach for the realization of 2D materials based nanoscale devices at wafer scale is discussed here. We begin with optimization of chemical exfoliation processes for the scalable production of high-quality thin-layers of graphene oxide (GO) and molybdenum disulphide and use it as a source for the realisation of versatile thin-films over arbitrary substrates. In an exemplary study, silicon and glass wafers are surface modified with different anchoring molecules using sophisticated gas-phase molecular deposition techniques. GO and MoS_2 flakes were then spin-coated over the surface modified wafers from their solutions in order to make homogeneous thin-films. Thin-films of GO and MoS_2 thin-films prepared thus are characterized using state-of-the-art surface characterization techniques and validated.

Further GO and MoS_2 thin-films are structured using routine photolithography and nanoimprint lithography techniques. A scalable and cost-effective techniques based on the use of chemically derived nanomaterial may offer numerous opportunities for the realization of different device platforms. Focussing towards the development of label-free sensor platform we use the GO and MoS_2 thin-films for the preparation of optical and electrical sensor platforms for the detection of biomolecules providing an alternative for otherwise expensive sensor fabrication processes.

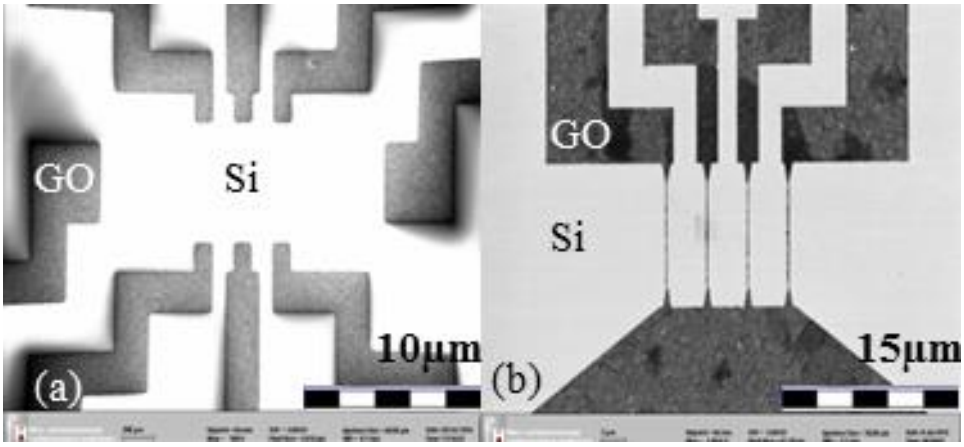

Figure 1 Chemically derived Graphene oxide thin-films are shown here structured using photolithography and nanoimprint lithography methods.

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24 Low-frequency raman spectroscopy of 2H and 3R transition metal dichalcogenides

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Transition metal dichalcogenides (TMDs) have attracted much attention due to their exceptional electronic and optical properties. Reliable synthesis and characterisation of these materials must be developed if these properties are to be exploited. Raman spectroscopy can be used to reveal a wealth of information about 2D materials in a fast and non-destructive manner. In particular, investigation of the low-frequency shear modes (SM) and layer-breathing modes (LBM) has been suggested as a universal method of layer number determination and characterisation of 2D materials.

Here, Raman spectra are acquired over large areas allowing changes in the position and intensity of the shear and layer-breathing modes to be visualised in maps. This allows detailed characterisation of mono- and few-layered TMDs, which is complementary to well-established (high-frequency) Raman and photoluminescence spectroscopy. This study also allows the identification of stacking configuration in these materials which we demonstrate for various 2H and 3R stacking orders up to 4 layers. This allows the quality, symmetry, stacking configuration and layer number of 2D materials to be probed over large areas.

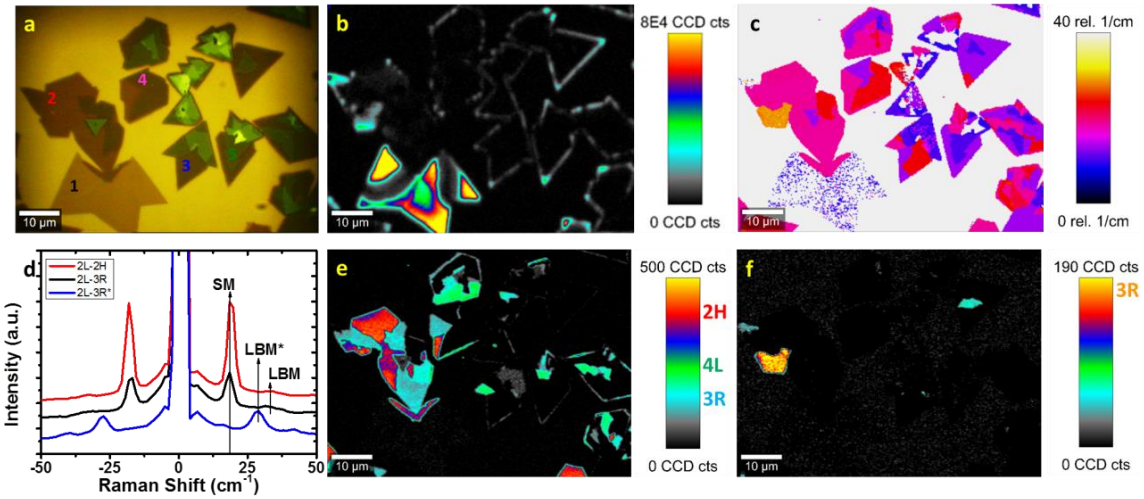

Figure 1 (a) Optical image of CVD $MoSe_2$. (b) Photoluminescence map. (c) Position of maximum in low frequency region. (d) Low-frequency Raman spectra of SMs and LBMs of 2H and 3R stacking configurations in 2L $MoSe_2$. (e) Peak intensity map for 2L $MoSe_2$ SM at ~18 cm^{-1}. (f) Peak intensity map for 2L $MoSe_2$ LBM at ~29 cm^{-1}.

[1] M. O'Brien, N. McEvoy *et al.*, "Mapping of Low-Frequency Raman Modes in CVD-Grown Transition Metal Dichalcogenides: Layer Number, Stacking Orientation and Resonant Effects", *Scientific Reports,* **6** (2016), 19476.

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25 Fabrication and optical properties of transition metal dichalcogenide heterostructures

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Semiconductor transition metal dichalcogenides (TMDs) have been subject of increasing interest over the last years. In particular single layers of molybdenum (or tungsten) disulfide (or diselenide) show strong photoluminescence associated with a direct-gap transition, in contrast to bulk. Heterostructures of TMDs will lead to modifications of their individual optical properties. Calculations predict that the band alignment of different monolayer TMDs is, for many combinations, of type II, leading to spatially indirect excitons. Nevertheless, clear experimental evidence is still missing.

Here we present our results on the influence of heterostructure fabrication on their optical properties. We used a dry transfer method, using a polymer stamp as an intermediate substrate, as proposed in [1]. The optical properties are investigated by Raman and photoluminescence spectroscopy. We studied few-layer MoS_2 obtained by stacking individual layers, and heterostructures of $MoSe_2$ and WS_2. Several cleaning methods have been considered to have proper interfaces with interacting layers. The cleanness of the layers, the influence of the transfer method as well as the influence of the substrate are analyzed.

This work was supported by the European Research Council (ERC) under grant number 259286.

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26 EELS probing of lithium based 2D battery compounds processed by liquid phase exfoliation

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Two-dimensional lithiated nanosheets usually show excellent electrochemical performance due to an increase in surface area and shorter diffusion paths. However, processing techniques, such as shear mixing or liquid phase exfoliation could induce phase changes or knock out some of the structural lithium (Li) ions, what in turn might result in poor electrochemical performance. Here different lithiated layered compounds mainly $LiCoO_2$, $LiMn_2O_4$, and $Li_5Ti_4O_{12}$ were chemically exfoliated and investigated using electron energy loss spectroscopy (EELS) for their Li-K edge. Further analyses were carried out, looking at the oxygen (O) K edge with their respective transition metal core loss peak (Mn, Co and Ti) which revealed changes in the Energy loss near edge structures (ELNES) when compared to the unlithiated compounds. STEM-EELS analyses confirmed uneven distribution of lithium within the lithiated layered materials. In this work, EELS was used for the first time to detect and to probe the chemical environment of the lithium in liquid phase exfoliated material.

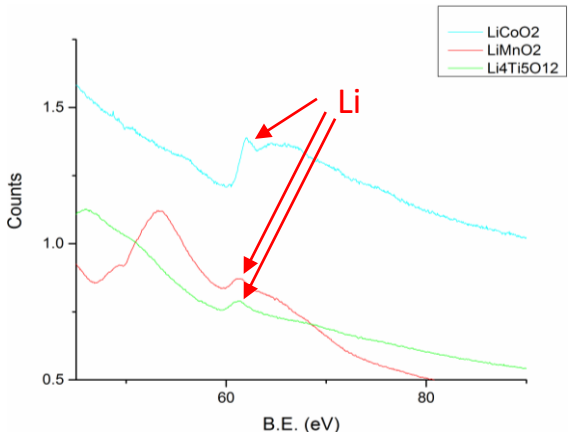

Figure 1 The EELS signals of all the materials examined showing the presence lithium (red arrows). Other reference spectra of MnO_2, cobalt oxide and titanium oxide.

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27 Liquid phase exfoliation and stability of monolayer TiS_2

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Transition metal dichalcogenides (TMDs) are layered materials with strong in-plane and weak out-of-plane bonds, which allow isolation of their elementary building blocks in the form of triatomic layers.

Among these materials, bulk TiS_2 has been employed as cathode in rechargeable batteries and it is now subject to renewed interest due to the possibility of being nanostructured in individual atomic layers.

In this work, we have obtained TiS_2 nanosheets through lithium intercalation followed by exfoliation in water.

We have studied the properties of exfoliated TiS_2 flakes and developed a methodology for characterising the number of layers with Raman spectroscopy. TiS_2 nanosheets have previously been shown to be unstable with rapid conversion to TiO_2. Here we study the kinetics of TiO_2 formation, propose methods of stabilising TiS_2 nanoflakes in suspensions, and we present prospective applications of stabilized nanostructured TiS_2 films.

28 Synthesis of new inorganic nanotubes

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Since the discovery of WS_2 nanotubes, inorganic nanosized structures have gained significant scientific and technological interest due to their unique physical, chemical and optical properties. WS_2 nanotubes can be considered as nanostructures originated by the bending of a single layer along one axis that gives origin to the characteristic high aspect-radio morphology typical of these species. This idea can be easily extended to other layered compounds, including chalcogenides, oxides and phosphates producing plenty of nanostructures with different properties. These nanostructures can be prepared following different synthetic protocols based on high temperature reaction, including for example CVT, solar (or laser) ablation and hydrothermal synthesis.

In this context we are studying the synthesis of new nanotubes based on layered WO_3-like oxides and metal iodates. These compounds are typically prepared by hydrothermal route, which presents various advantages from the synthetic point of view, such as reduced costs and an easy implementation in multigram scale. These synthetic protocols can be easily modified by the introduction of suitable organic molecules that could act as structure directing agents during the precipitation, yielding inorganic nanotubes. This strategy has been applied to quaternary WO_3-like oxides, which are characterized by second harmonic generation and piezoelectric properties, due to the presence of capping groups orthogonally aligned in respect of the crystal layers.

The synthesis of metal iodate nanotubes is interesting both by the application and the fundamental point of view since this kind of structure has not been reported so far. Interestingly the crystal structures of these compounds are characterized by the lack of the centrosymmetric element, giving rise to second order non-linear properties.

The materials have been characterized by X-ray diffraction, TEM and SEM microscopy.

29 Palladium coatings for prevention of bacterial infection

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Biocompatible polymers are suitable materials for medical devices, such as catheters, endotracheal tubes, stents and prosthesis[1,2]. However, the use of untreated medical devices can lead to severe hospital-acquired infections. The most frequent types of these complications are pneumonia, surgical site infection, urinary tract and bloodstream infection, all of which are very often caused by Gram-negative bacteria[3].

Pd nanolayers of variable thicknesses ranging from 0.4 to 22.4 nm were prepared by sputtering technique on polyethylene naphthalate (PEN). Low-temperature annealing was applied to transform these nanolayers into discrete nanoislands homogeneously distributed over the surface of the underlying polymer. The antibacterial properties of such composites (both thin metal coatings and discrete nanoislands supported on PEN) were evaluated by drip test using Gram-positive and Gram-negative bacteria as model strains. *In vitro* cytotoxicity assessment of Pd nanostructures was performed by WST-1 assay and cell viability was determined. Finally, cell morphology in response to Pd/PEN interface was evaluated by fluorescence microscopy.

Inductively coupled plasma, X-ray photoelectron spectroscopy, and atomic force microscopy were used to outline the way of bacterial inhibition by Pd nanostructures. We found that the antibacterial effect of the Pd/PEN composites originate from both i) release of Pd into a physiological solution and ii) direct contact of bacteria with the Pd interface. Our results suggest that the samples coated with 22.4 nm thick Pd layer exhibited significantly enhanced antibacterial properties compared to the thinner Pd coatings (see Figure 1).

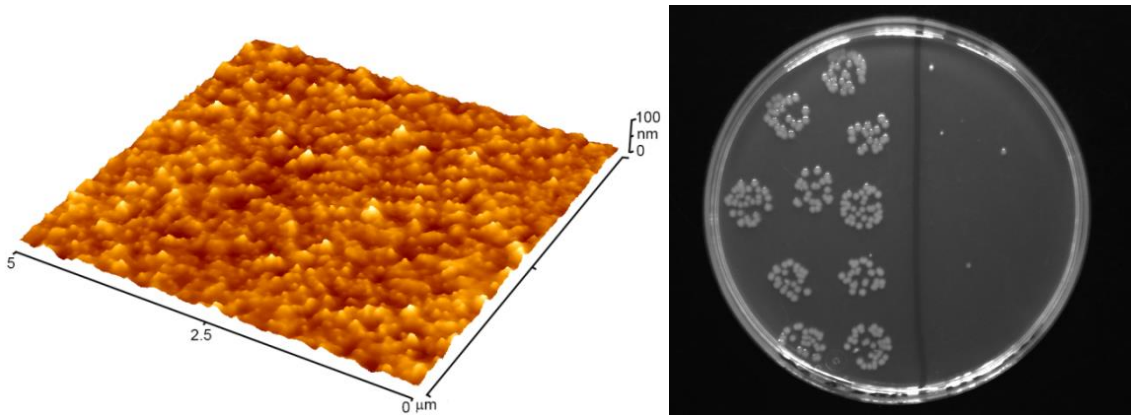

Figure 1 AFM scan of 22.4 nm thick Pd layer on PEN (left) with Photograph showing the inhibition effect of Pd-coated PEN on *E. coli* (right).

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30 Unlocking the functional properties in one-dimensional MoSI cluster polymers by doping and photoinduced charge transfer

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To improve functionalization of MoSI cluster polymers we have studied the effects of adsorption doping on the electrical transport, bundling, and optical absorption spectra. Doping results both in enhanced conductivity and aggregated bundles in dispersion. The different electronic properties of different bundle diameters can be ascribed to self-doping during the synthesis. Furthermore, doping shifts the characteristic absorption peaks and transfers oscillator strength to lower energies. Femtosecond optical spectroscopy shows that the spectral signature of adsorption and self-doping indeed originates from the population of electronic levels that are empty or absent in the undoped sample. The large spectral shifts and long lifetimes of photoinduced charges suggest efficient localization.

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31 Exfoliated MoS_2 and WS_2 as charge selective layers in perovskite solar cells

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Perovskite solar cells are firmly considered as the fastest developing photovoltaic technology up to date, nowadays with power conversion efficiencies surpassing 20%[1,2]. The performance leap achieved in a matter of a few years can be assigned to various factors, particularly to the smart processing and compositional engineering of perovskite as well as to the use of novel organic materials applied as a charge extracting layers. However, some mostly used organic layers, besides being limited in the choice of deposition techniques, show degradation under prolonged exposure to high temperatures. To avoid these problems we present the use of exfoliated transition metal dichalcogenides as charge extracting layers in perovskite solar cells. We focus on exfoliated two-dimensional MoS_2 and WS_2 layers that are deposited in an ultra thin manner, conforming to the surface of the substrate or the active layer, thus reducing the material consumption and series resistance in a device. Additional doping of layers is applied to provide favorable band alignment with perovskite layer and better charge selectivity.

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32 Helical Raman and photoluminescence spectroscopy of transition metal dichalcogenides

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Transition metal dichalcogenides (TMDs) have attracted a lot of interest due to their unique properties. Especially the strong photoluminescence from the direct gap in few-layered samples has been repeatedly investigated. Furthermore, TMDs have recently become promising materials for spin- and valleytronics as circular polarized excitation leads to the generation of electron-hole pairs with distinct spin at either K or K'. However, questions remain unanswered about the mechanisms of the scattering processes, especially on phonons.

We have performed circular polarization resolved Raman and photoluminescence spectroscopy with different excitation energies. We will present the observed differences in polarization conservation and discuss the resonance behavior of the conservation.

33 Optical properties of GaS-Ca(OH)$_2$ bilayer heterostructure

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Investigating characteristic physical properties of novel atomically-thin heterostructures is crucial for the nanoscale optoelectronic devices. In this study, we investigate the electronic and the optical properties of GaS-Ca(OH)$_2$ heterobilayer using density functional theory (DFT). Both of the constituent monolayers are recently synthesized and wide band gap semiconductors. The band gap of the heterobilayer drastically reduces when compared with those of the isolated constituent layers. Our band alignment calculations show that the GaS-Ca(OH)$_2$ heterobilayer is a type-II heterojunction in which the conduction and the valence band edges originate from GaS and Ca(OH)$_2$ monolayers, respectively. Therefore, the heterobilayer can be used to separate photoinduced charge carriers where electrons are localized in GaS and holes in the Ca(OH)$_2$ layers which leads to have spatially indirect excitons.

By solving the Bethe-Salpeter equation on top of single shot GW calculation (G0W0) the dielectric function and optical oscillator strength of the constituent monolayers and the heterobilayer are obtained. The oscillator strength of the optical transition for GaS monolayer is an order of magnitude larger than the Ca(OH)$_2$ monolayer. We also found that the calculated optical spectra of different stacking types (*i. e.* transmittance and reflectivity) of the heterobilayer show dissimilarities, although their electronic structures are rather similar as shown in Figure 1. This prediction can be used to determine the stacking type of ultra-thin compounds[1].

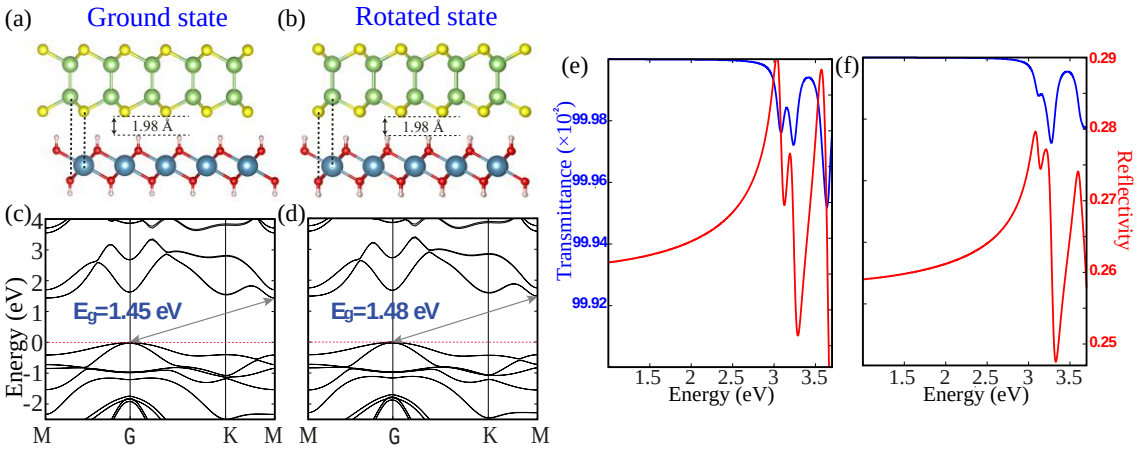

Figure 1 The optimized geometric structures of the two configurations of the GaS-Ca(OH)$_2$ heterobilayer: (a) Ground and (b) rotated state, which is 5 meV higher in energy. Their electronic structure (c,d) and optical transmittance (e) and reflectivity (f).

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34 Real-time observation of phase transition to the hidden quantum state in 1T-TaS_2 by optical time-resolved spectroscopy

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Increasingly more difficult computational tasks in various fields require further development of supercomputer capabilities. Although the CPU speeds are approaching the Moore's limit, they are still improving significantly, while read/write speeds of memory devices are lagging behind, thus limiting the overall performance of the computer.

Recently, it was shown that the new type of memory devices based on the phase transition to the hidden quantum state in charge-density wave (CDW) material 1T-TaS_2 can provide the desired and necessary memory speed improvement. While the switching was observed after a single 35-fs laser[1] or 40-ps electrical pulse[2], there was no direct information on the real-time speed of the transition itself.

I will present the results of a multi-pulse optical time-resolved study of the phase transition between the ground and the hidden state in 1T-TaS_2. Our data proves that the transition occurs within one oscillation period of the collective mode of CDW. The modeling predicts that the final state of the sample can be controlled coherently, which will provide additional prospects for implementation of the effect in memory devices.

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35 Patterning photonic structures by soft lithography in WS_2 PMMA composite

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Liquid phase exfoliation has been proven as a successful method for production of transition metal dichalcogenide dispersions[1]. In order to produce devices these liquid dispersions need to be processed into solid assemblies. This work shows how to transfer WS_2 monolayer enriched dispersions to polymer/solvent dispersion and deposit them in a microstructured thin composite film.

Soft lithography[2] was used to obtain a homogeneous pattern in a large area surface. Commercial DVD masters were used to fabricate a PDMS stamp. Two different substrates were tested (SU8 and SiO_2). On both samples, 5 µl of resist was drop cast. The resist is then covered with the PDMS stamp and pressed between two glasses. The resist is cured under vacuum for 3 hours. After the patterning procedure, the photoluminescence of the treated material is preserved.

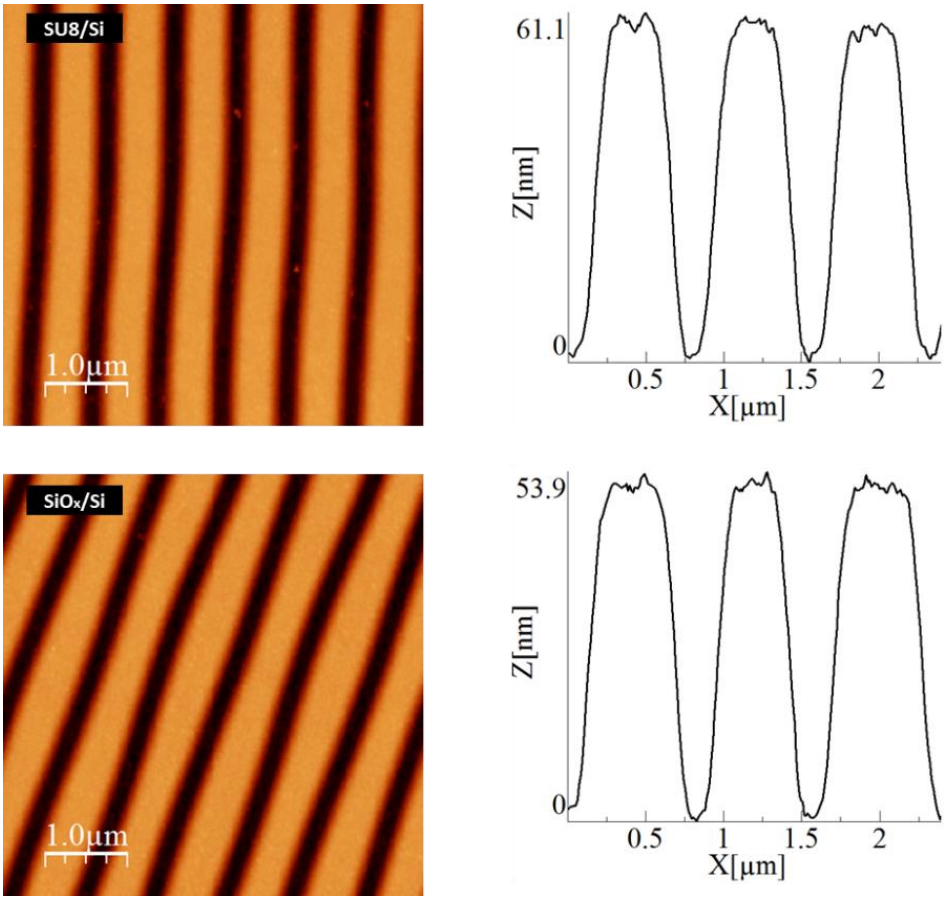

Figure 1 AFM images of resist pattern on SU8 and SiO_x on silicon sample.

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36 P-type MoS_2 thin film transistors fabricated from liquid phase

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In this work, MoS_2 films obtained from precursor solution *via* spin-coating on various substrates were investigated. Molybdenum(V)-chloride dissolved in organic solvent was spin-coated on silicon/silicon-dioxide substrates and also on sapphire to form uniform and closed films over large area (2 cm × 2 cm). The MoS_2 films were obtained after annealing in presence of sulfur. Deposited films were analyzed for surface morphology and roughness, chemical composition and crystallinity. In addition, influence of substrate orientation on film growth will be discussed, together with effect of processing conditions (environment, moisture, etc.) on film composition and film quality. The thickness of the MoS_2 films was controlled in the process, and we have observed that film thickness linearly scales with precursor concentration, thereby resulting in film thicknesses between 4 nm and 27 nm. All MoS_2 films performed with low surface roughness below 1.5 nm. SEM/EDX and XRD measurements indicate that the film morphology, composition, and crystallinity are dependent on the annealing temperature. Temperatures above 750 °C are needed for effective MoS_2 film formation. This novel approach allows low-cost deposition of MoS_2 films compared to the current state-of-the-art chemical vapour deposition technique[1].

On top of solution processed MoS_2 films, gold layer was deposited by e-beam evaporation using a shadow mask to define source and drain contacts of thin film transistors (TFTs). Fabricated TFTs exhibited gate dependence and p-type semiconducting behaviour with field-effect mobility as high as 0.1 cm^2/Vs. Furthermore, scaling of the film thickness and different processing temperatures have an effect on the grain size and thus on TFT performance. The future steps will lead towards improvement of the TFT performance and its application in various electronic devices (displays, inverters, sensors, etc.).

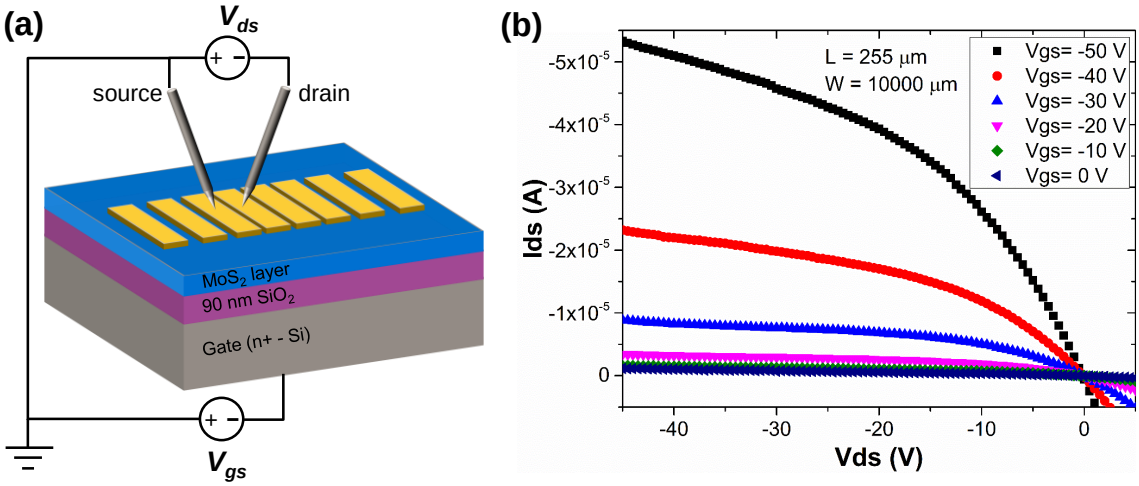

Figure 1 (a) The TLM structure is used for electrical characterization of MoS_2 films. (b) The output characteristic of solution processed MoS_2-TFT.

[1] Jeon, J. *et al.* Layer-controlled CVD growth of large-area two-dimensional MoS_2 films. *Nanoscale* **7,** 1688–1695 (2015).

37 TFT fabrication based on liquid-exfoliated MoS_2 flakes

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There is a large interest in establishing cheap, scalable processes for producing low-dimensional semiconducting dichalcogenide films for electronic application. In this work, well exfoliated MoS_2 dispersions were prepared through two-step liquid phase exfoliation process with N-methyl-pyrrolidone (NMP) and isopropanol (IPA). The obtained exfoliated MoS_2 flakes were characterized by microscopy (TEM and SEM), UV-Vis and Raman spectroscopy.

Bottom-gate thin film transistors (TFTs) based on exfoliated MoS_2 films were fabricated by using spray coating techniques. The deposition process was optimized to get uniform and percolated MoS_2 films with different thicknesses. Directly after layer deposition, transistors show minor conductivity. However, depositing additional PMMA layer on top shows large improvement in electrical characteristics, *i. e.* proper switching behavior with changing gate voltage. Interpretation is that the PMMA layer improves the inter-flake contact and enables proper percolation. This low-cost and scalable solution-based fabrication process will promote the application of dichalcogenides in future nanoelectronic devices.