CECAM – Workshop

Tailor-made 2D-materials and functional devices

June 27th – July 1st 2016

Bremen Center for Computational Materials Science

University of Bremen

Program of the International CECAM-Workshop
"Tailor-made 2D-materials and functional devices"

Bremen Center for Computational Materials Science – BCCMS
University of Bremen, June 27th – July 1st 2016
Conference site: House of Science, Downtown

Monday, June 27th 2016 (RAMADA Ueberseehotel Bremen)

18:00	**–**	**21:00**	**Registration**

Tuesday, June 28th 2016 (House of Science Bremen, Downtown)

08:00	**–**	**08:50**	**Registration**
08:50	**–**	**09:00**	**Opening and welcome, Thomas Frauenheim**
Session:			**Carbon and other hexagonal nanostructures**
			Chair: Young Hee Lee
09:00	**–**	**09:40**	Zhongfan Liu, Beijing University, China *2D nanocarbons: a road towards controlled growth*
09:40	**–**	**10:20**	Takashi Taniguchi, National Institute for Materials Science, Tsukuba, Ibaraki, Japan *Synthesis & properties of hexagonal boron nitride single crystals*
10:20	**–**	**10:50**	**Coffee Break**
10:50	**–**	**11:30**	Zhongfang Chen, University of Puerto Rico, San Juan, US *Planar hypercoordinated carbon in 2D materials*
11:30	**–**	**12:10**	Hannu-Pekka Komsa, Aalto University, Finland *Defects in 2D materials: their production under irradiation, evolution and properties from 1st principles*
12:10			**Group photo**
12:15	**–**	**14:00**	**Lunch Break (Restaurant Stadtwirt) and Coffee**
Session:			**Topology and superconductivity**
			Chair: Tim O. Wehling
14:00	**–**	**14:40**	Jinfeng Jia, Shanghai Jiao Tong University, China *Epitaxial growth of two-dimensional stanene and artificial topological superconductors*
14:40	**–**	**15:20**	Binghai Yan, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany *Discovery of a new type of topological Weyl semimetal in the layered transition metal dichalcogenide MoTe2*
15:20	**–**	**15:50**	**Coffee Break**
15:50	**–**	**16:30**	Elena Roxana Margine, Binghamton University, New York, US *Superconducting carbon in two dimensions*
16:30	**–**	**17:10**	Gunnar Schoenhoff, University of Bremen, Germany *Coulomb interaction in transition metal dichalcogenides: effects on many-body instabilities*
17:10	**–**	**17:50**	Yong Xu, Tsinghua University, Beijing, China *Recent research progress of two-dimensional stanene*
19:00	**–**	**21:30**	**Welcome Reception (Bremen Town Hall)**

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Wednesday, June 29th 2016 (House of Science Bremen, Downtown)

Session:			**Topology and superconductivity (continued)**
			Chair: Hannu-Pekka Komsa
09:00	–	**09:40**	Alexander Steinhoff, University of Bremen, Germany *Optical properties and carrier dynamics in transition metal dichalcogenides*
09:40	**–**	**10:20**	Thomas Heine, Leipzig University, Germany *Strong quantum confinement and topological phases in two-dimensional crystals*
10:20	**–**	**10:50**	**Coffee Break**
Session:			**TMDCs: optical properties and carrier dynamics**
10:50	**–**	**11:30**	Michael Rohlfing, University of Muenster, Germany *Optical spectra of atomically thin semiconductors from ab-initio many-body perturbation theory*
11:30	**–**	**12:10**	Isabella Gierz, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany *Electron dynamics in low dimensions: a time- and momentum-resolved view*
12:10	**–**	**14:00**	**Lunch Break (Restaurant Stadtwirt) and Coffee**
Session:			**TMDCs: optical properties and carrier dynamics (continued)**
			Chair: Yandong Ma
14:00	**–**	**14:40**	Christoph Gadermaier, Jožef Stefan Institute, Ljubljana, Slovenia *Femtosecond exciton and charge dynamics and unusual Stark effect in mono- and few-layer transition metal dichalcogenides*
14:40	**–**	**15:20**	Sean C. Smith, University of New South Wales, Sydney, Australia *Electrocatalytic gas capture on 2D nanomaterials*
15:20	**–**	**15:50**	**Coffee Break**
15:50	**–**	**16:30**	Jonathan Finley, Technical University of Munich, Germany *Electrical control of the optical response of atomically thin semiconductors*
16:30	**–**	**17:10**	Ji-Hee Kim, Sungkyunkwan University, Suwon, South Korea *Ultrafast exciton dynamics in 2D TMDC materials*
18:40			**Bus Pickup to Conference Dinner** (Pick-up Venue: RAMADA Ueberseehotel Bremen)
19:00	**–**	**22:30**	**Conference Dinner (Restaurant Juergenshof)**

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Thursday, June 30th 2016 (House of Science Bremen, Downtown)

Session:			**Hetero-structures and devices**
			Chair: Beata Kardynal
09:00	**–**	**09:40**	David Abergel, Nordita, KTH Royal Institute of Technology and Stockholm University, Sweden *Two-dimensional lateral heterostructures*
09:40	**–**	**10:20**	Young Hee Lee, Sungkyunkwan University, Suwon, South Korea *Controlling contact resistance in 2D layered materials*
10:20	**–**	**10:50**	**Coffee Break**
10:50	**–**	**11:30**	Hyun Seok Lee, Sungkyunkwan University, Suwon, South Korea *Tunable optical and electrical properties in 2D semiconductors and their optoelectronic applications*
11:30	**–**	**12:10**	Tony F. Heinz, Stanford University, California, US *Optical properties of 2D semiconductors and hetero-structures*
12:10	**–**	**14:00**	**Lunch Break (Restaurant Stadtwirt) and Coffee**
Session:			**Hetero-structures and devices (continued)**
			Chair: Gotthard Seifert
14:00	**–**	**14:40**	Aijun Du, Queensland University of Technology, Brisbane, Australia *Predicting new 2D materials and exploring the possible applications in energy conversion*
14:40	**–**	**15:20**	Heejun Yang, Sungkyunkwan University, Suwon, South Korea *Novel 2D interfaces with silicon, graphene, MoTe2 and Ca2N*
15:20	**–**	**16:00**	Dong Hee Son, Texas A&M University, College Station, US *Photoluminescence and polarization properties of colloidal single layer TMDC quantum dots*
17:25			**Poster Mounting**
17:30	**–**	**20:30**	**Poster Session, Catering Dinner (House of Science)**

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Friday, July 1st 2016 (House of Science Bremen, Downtown)

Session:			**TMDCs: electronic properties**
			Chair: Thomas Brumme
09:00	**–**	**09:40**	Biplab Sanyal, Uppsala University, Sweden *Functional 2D transition metal dichalcogenides: defects, adsorption and magnetism*
09:40	**–**	**10:20**	Gianluca Fiori, University of Pisa, Italy *Multi-scale modelling of devices based on two-dimensional materials*
10:20	**–**	**10:50**	**Coffee Break**
10:50	**–**	**11:30**	Agnieszka-Beata Kuc, Leipzig University, Germany *Modulation of electronic structure in low-dimensional transition-metal dichalcogenides*
11:30	**–**	**12:10**	Michael Bauer, University of Kiel, Germany *Electronic structure and dynamics at surfaces of 2D TMDCs*
12:10	**–**	**12:50**	Gotthard Seifert, Dresden University of Technology, Germany *Layered nanostructures - electronic and mechanical properties*
12:50	**–**	**13:00**	**Closing remarks: Tim O. Wehling**
13:00			**Departure**

Abstracts of Lectures

2D nanocarbons: a road towards controlled growth

Zhongfan Liu

Peking University, Center for Nanochemistry, Beijing Science and Engineering Center for Nanocarbons, College of Chemistry and Molecular Engineering, Beijing, China

Carbon element has a great number of allotropes, covering the traditional three dimensional (3-D) diamond and graphite, 2D graphene, 1D carbon nanotubes and 0-D fullerenes. Recently, graphyne, a new 2D carbon allotrope family formed by sp and sp2 hybridization carbon atoms also comes into the stage. Theoretical calculations further indicate that there may exist a penta-graphene, formed by a huge number of carbon pentagons in a 2D fashion instead of the hexagon structure of graphene. Therefore, 2D nanocarbons including graphene, graphyne, etc have created a new category of carbon allotropes which attract increasing attentions. We have been working on the controlled synthesis of 2D nanocarbons for many years. Systematic studies have been done on the chemical vapor deposition (CVD) of high quality graphene on various solid substrates ranging from metals (Cu, Ni, Cu-Ni alloy, Pt, Ru, Rh, Ir, Pd), groups IV-VI early transition metal carbides, to dielectric substrates (h-BN, STO, glass, NaCl). We also made a great effort for the controlled synthesis of graphdiyne, a representative member of the graphyne family. A brief overview will be made in the talk following a general concept of CVD process engineering by highlighting the catalyst design, super graphene glass and scalable production techniques of graphene and various applications as well as the Glaser-Hay coupling synthesis of graphdiyne nanowalls on Cu foils and foams.

Synthesis & properties of hexagonal boron nitride single crystals

Takashi Taniguchi

National Institute for Materials Science, Sengen, Japan

The attractive potential of hexagonal boron nitride (hBN) as a wide-band gap material was realized after obtaining high quality single crystals by using Ba-BN as a growth solvent material at high pressure (HP) of 5.5GPa. Band-edge natures (hBN Eg=6.4eV) were characterized by their optical properties, while the key issue to obtain high purity crystals is to reduce oxygen and carbon contamination in the HP growth circumstances. Taking advantage of the highly luminous properties of hBN, a stable operation of far ultraviolet -plane-emission device was demonstrated. It is also emphasized that hBN crystals exhibits superior properties as a substrate of graphene devices. In order to realize these newly developed potential of hBN crystals, development of synthesis route of high quality crystals at ambient conditions and further insight for its quality control may be important issue.

Although the major impurities affects the optical properties of hBN are carbon and oxygen, the details of their contribution are still not well known. In order to figure out this issue, this paper focus on a spatial distribution of residual carbon impurity within hBN single crystals and modification of their properties depend upon post heat treatments.

On the other hands, liquid phase crystal growth process is applicable for other 2D materials such as graphite, black phosphor (BP) and TMDs such as MoS_2, WS_2, WSe_2. In this paper, recent our trials of crystal growth for hBN, graphite, BP and TMDs at high pressure will be also introduced.

Planar hypercoordinated carbon in two-dimensional materials

Zhongfang Chen

University of Puerto Rico, Department of Chemistry, San Juan, Puerto Rico, USA

Rule-breaking molecules not only enrich chemical bonding theory, gain us deeper chemical insights, but also often lead to discoveries of exceptional materials with novel properties. Molecules with planar hypercoordinate carbon are seminal examples.

Here by means of density functional theory (DFT) computations, we extend the planar hypercoodinate carbon from molecules to two-dimensional nanomaterials. Our predicted SiC_2, Al_2C, Be_2C and Be_5C_2 monolayers have rather unusual chemical bonding: the Si/C atoms in SiC_2/Al_2C adopt planar tetracoordinate configuration, while Be_2C/Be_5C_2 contains planar hexa-/penta-coordinate carbon moieties. Besides the unique bonding character, these rule-breaking systems also hold great promise for applications in nanoelectronics, photoelectronics, and mechanics. For example, our newly predicted Be_5C_2 monolayer is a gapless semiconductor with a Dirac-like point in the band structure, and also has an unusual negative Poisson's ratio. The high stabilities of these systems strongly suggest the feasibility for their experimental realizations. We are calling for more efforts on nanomaterials with novel chemical bonding, especially on the rule-breaking systems.

Defects in 2D materials: their production under irradiation, evolution, and properties from first principles

Hannu-Pekka Komsa, Arkady V. Krasheninnikov

Aalto University, Department of Applied Physics, Aalto, Finland

Two-dimensional (2D) materials such as graphene, hexagonal boron nitride, and transition metal dichalcogenides (TMDs) have recently received lots of attention due to their unique properties and numerous potential applications. All these materials have defects, which naturally affect their characteristics. Moreover, defects and impurities can deliberately be introduced by irradiation or chemical treatment to tailor the properties of these systems.

In my talk, I will present the results of our first-principles theoretical studies [1-7] of defects in 2D systems, compare them to the experimental transmission electron microscopy data, and discuss how defect and impurities can be used to engineer the electronic structure of 2D materials. Specifically, we showed that vacancies in TMDs produced by the electron beam agglomerate and form line structures, which can be used for engineering material properties [2]. In some chalcogen-deficient TMDs, rotational defects appear under electron beam [4], which eventually give rise to formations of new grains inside the material. We further demonstrated that TMDs can be doped by filling the vacancies with impurity atoms or introducing impurities during the growth stage [1,3].

We also studied the atomic scale morphology of non-stoichiometric TMD $MoSe_{(2-x)}$ and showed that a Se-deficit in single layers of $MoSe_2$ grown by molecular beam epitaxy gives rise to a dense network of mirror-twin-boundaries (MTBs) decorating the 2D-grains [5]. Using density functional theory calculations, we further demonstrated that MTBs are thermodynamically stable structures in Se-deficient sheets. These line defects host localized states close to the valence band minimum thus giving rise to enhanced conductance along straight MTBs.

On the other hand, in 2D materials with anisotropic atomic structure, defect stability and dynamics can present distinct features. For instance, in ReS_2 the vacancies are seen to be preferentially produced at certain chalcogen sites [6]. These sites, located between the Re diamond chains, also exhibit lowest formation energy. Finally, we computationally predicted the irradiation stability of pristine phosphorene, traced the first steps in damage evolution, and studied the defect dynamics [7].

References

[1] H-P. Komsa, J. Kotakoski, S. Kurasch, O. Lehtinen, U. Kaiser, and A. V. Krasheninnikov, Phys. Rev. Lett. 109, 035503 (2012).

[2] H.-P. Komsa, S. Kurasch, O. Lehtinen, U. Kaiser, and A. V. Krasheninnikov, Phys. Rev. B 88, 035301 (2013).

[3] Y.-C. Lin, D.O. Dumcenco, H.-P. Komsa, Y. Niimi, A.V. Krasheninnikov, Y.-S. Huang, and K. Suenaga, Advanced Materials 26, 2857 (2014).

[4] Y.-C. Lin, T. Björkman, H.-P. Komsa, F.-S. Huang, C.-H. Yeh, K.-H. Lin, J. Jadczak, Y.-S. Huang, P.-W. Chiu, A. V. Krasheninnikov, K. Suenaga, Three-fold rotational defects in two-dimensional transition metal dichalcogenides, Nature Commun. 6, 6737 (2015).

[5] O. Lehtinen, H.-P. Komsa, A. Pulkin, M.B. Whitwick, M.-W. Chen, O.V. Yazyev, A. Kis, U. Kaiser, and A.V. Krasheninnikov, ACS Nano 9, 3274 (2015).

[6] Y.-C. Lin, H.-P. Komsa, C.-H. Yeh, T. Björkman, Z.-Y. Liang, C.-H. Ho, Y.-S. Huang, P.-W. Chiu, A. V. Krasheninnikov, K. Suenaga, Single-Layer ReS 2 : Two-Dimensional Semiconductor with Tunable In-Plane Anisotropy, ACS Nano 9, 11249 (2015).

[7] V. Vierimaa, A. V. Krasheninnikov, H.-P. Komsa, Phosphorene under electron beam: from monolayer to one-dimensional chains, Nanoscale (2016), DOI: 10.1039/C6NR00179C

Epitaxial growth of two-dimensional stanene and artificial topological superconductors

Jinfeng Jia

Shanghai Jiao Tong University, Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Department of Physics and Astronomy, Shanghai, China

Ultrathin semiconductors present various novel electronic properties. The first experimental realized two-dimensional (2D) material is graphene. Searching 2D materials with heavy elements bring the attention to Si, Ge and Sn. Sn-based stanene has its unique properties. Stanene and its derivatives can be 2D topological insulators (TI) with a very large band gap as proposed by first-principles calculations, or can support enhanced thermoelectric performance, topological superconductivity and the near-room-temperature quantum anomalous Hall (QAH) effect. For the first time, in this work, we report a successful fabrication of 2D stanene by MBE. The atomic and electronic structures determined by STM and ARPES agree well with results by first-principles calculations. This work will stimulate the experimental study and exploring the future application of stanene. In the second part of the talk, I will discuss our recent efforts to make artificial topological superconductors by proximity effects and identify the Majorana mode in the vortex core. This work provides consistent evidences for the existence of Majorana fermions and also suggests a possible route to manipulating them.

Discovery of a new type of topological Weyl semimetal in the layered transition metal dichalcogenide $MoTe_2$

Binghai Yan

Max Planck Institute for Chemical Physics of Solids and Max Planck Institute for the Physics of Complex System, Dresden, Germany

The Weyl semimetal became a new frontier of topological materials since the discovery in solid-state compounds in 2015. We predicted the existence of a new type of Weyl semimetals in the transition-metal dichalcogenide $MoTe_2$ [1], which has been verified by ARPES recently [2]. In this talk, I will explain the topological feature in the $MoTe_2$ bulk band structure and the experimental hallmark, surface Fermi arc states. Further, we found that $MoTe_2$ exhibits large magnetoresistance and superconductivity in experiment, in which the superconducting Tc can be largely enhanced by external pressure [3]. The multifunctionality of $MoTe_2$ supplies a profound platform to study the interplay between topological states, superconductivity and magneto-transport properties.

References

[1] Sun, S. C. Wu, M. N. Ali, C. Felser, and B. Yan, PRB 92, 161107(R) (2015).
[2] J. Jiang, et al., arXiv:1604.00139 (2016).
[3] Y. Qi, et al., Nature Comm. 7, 11038 (2016).

Superconducting carbon in two dimensions

Elena Roxana Margine

Binghamton University, The State University of New York, Department of Physics, Applied Physics and Astronomy, Binghamton, New York, United States

Carbon is a wonder element which underpins life on our planet, represents the vast majority of our energy sources, and arguably constitutes one of the building blocks of nanotechnology. Among its many fascinating properties, carbon has been known to exhibit superconductivity in zero, one, and three dimensions in widely diverse materials spanning fullerenes, graphite, polycyclic aromatic hydrocarbons, nanotubes, and diamond. One outstanding question in this area has been whether carbon can also superconduct in strictly two dimensions, namely in graphene and its derivatives. Very recently, three independent studies have presented the first evidence supporting the appearance of a superconducting phase in Li-decorated monolayer graphene (LiC_6) [1], Ca-intercalated bilayer graphene (C_6CaC_6) [2], and Ca-intercalated graphene laminates [3].

In this talk I will review our recent computational work on the electron-phonon interaction and the paring mechanism in Ca-intercalated bilayer graphene [4] and Li-decorated monolayer graphene [5]. In both cases we provide evidence that the superconducting transition can be explained within a standard phonon-mediated mechanism and find that the low-energy vibrations associated with the alkali atoms are critical to the pairing. Finally, we predict that while a single anisotropic superconducting gap should exist in LiC_6, it should be possible to resolve two distinct superconducting gaps in C_6CaC_6. I will conclude this talk by discussing recent advances in first-principles calculations for superconductors, in particular our recent implementation of the anisotropic Eliashberg theory using Wannier-Fourier electron-phonon interpolation [6,7,8].

References

[1] B. M. Ludbrook et al., PNAS 112, 11795 (2015).
[2] S. Ichinokura et al., ACS Nano 10, 2761 (2016).
[3] J. Chapman et al., Sci. Rep. 6, 23254 (2016).
[4] E. R. Margine, H. Lambert, and F. Giustino, Sci. Rep. 6, 21414 (2016).
[5] J. Zheng and E. R. Margine, submitted (2016).
[6] E. R. Margine and F. Giustino, Phys. Rev. B 87, 024505 (2013).
[7] S. Poncé, E. R. Margine, C. Verdi, and F. Giustino, submitted (2016).
[8] http://epw.org.uk/

Coulomb interaction in transition metal dichalcogenides: effects on many-body instabilities

Gunnar Schoenhoff (1,2), Malte Roesner (1,2),
Stephan Haas (3), Tim Oliver Wehling (1,2)

(1) University of Bremen, Institute for Theoretical Physics, Bremen, Germany
(2) University of Bremen, BCCMS, Department of Physics, Bremen, Germany
(3) University of Southern California, Department of Physics and Astronomy, Los Angeles, California, USA

We develop a material realistic, microscopic model to describe the Coulomb interaction in a TMDC monolayer, focusing on molybdenum disulfide under electron doping. Starting from ab initio Coulomb interaction for the undoped system, we look at the freestanding layer and include substrates. Additionally, we obtain the doping dependent electron-phonon matrix elements and observe a Charge Density Wave instability at high doping.
To quantify the influence of the Coulomb interaction on the superconducting phase, we calculate the Morel-Anderson coefficient μ*. In contrast to the frequent use of μ* as a fit parameter or a constant, this leads to a decrease of μ* with electron doping. The influence of the Coulomb interaction turns out to be most important at the boundary between the metallic and the superconducting phase where it delays the phase transition. We argue that the character of the superconducting phase in MoS_2 is phononic.

Recent research progress of two-dimensional stanene

Yong Xu

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RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama, Japan

Stanene is a two-dimensional (2D) atomically thin sheet of tin in a buckled honeycomb lattice. In contrast to other 2D group-IV materials (including graphene, silicene and germanene), stanene is of special interest owing to its outstanding properties. Stanene and its derivatives could support many novel features, such as large-gap quantum spin Hall states [1], enhanced thermoelectric performance [2], topological superconductivity [3] and the near-room-temperature quantum anomalous Hall e ect [4]. Recent research progress of 2D stanene will be reviewed in this talk. In particular, as an important progress, a recent experiment has successfully fabricated monolayer stanene, which, for the first time, confirmed the existence of this theoretically predicted structure [5,6]. These preliminary progresses make the research of 2D stanene a fast-growing field, interesting for exploring low-dimensional and topology-related physics.

References

[1] Y. Xu et al. PRL 111, 136804 (2013).
[2] Y. Xu et al. PRL 112, 226801 (2014).
[3] J. Wang, et al., Phys. Rev. B 90, 054503 (2014).
[4] S.-C. Wu, et al., Phys. Rev. Lett. 113, 256401 (2014).
[5] F. Zhu, W.-J. Chen, Y. Xu, et al., Nature Mater. 14, 1020 (2015).
[6] Y. Xu et al., Phys. Rev. B 92, 081112(R) (2015).

Optical properties and carrier dynamics in transition metal dichalcogenides

Alexander Steinhoff, Matthias Florian, Malte Roesner, Michael Lorke,
Ji-Hee Kim, Deok-Soo Kim, Chanwoo Lee, Gang Hee Han,
MunSeok Jeong, Christopher Gies, Tim Wehling, Frank Jahnke

Universität Bremen, Institute for Theoretical Physics, Bremen, Germany

Monolayers of transition metal dichalcogenide semiconductors have been in the spotlight due to direct optical transitions in the visible spectral range and exciton binding energies of ~500 meV.
In particular, there is a strong interest in understanding the influence of excited carriers on optical properties. On the theory-side, ab-initio electronic state calculations provide ground-state single-particle properties and their combination with numerical solutions of the Bethe-Salpeter equation determines the excitonic ground-state absorption. We extend these investigations by studying optical properties in the presence of excited carriers as well as relaxation kinetics.
It is shown that absorption spectra are strongly modified due to band-gap renormalization and screening of the Coulomb interaction under the influence of excited carriers, while the photoluminescence signal can be distinctly influenced by optical excitation above or below the electronic band gap. Moreover, the role of strain and the corresponding modifications of the band structure are studied, leading to a characteristic reduction of emission in certain situations.
For investigations of the carrier dynamics in MoS_2 we present results for the carrier-carrier Coulomb scattering and carrier-phonon scattering after optical excitation of the monolayer. As for the optical spectra, these investigations are based on ab-initio band structure and interaction matrix elements and reveal ultrafast relaxation of excited carriers.

Strong quantum confinement and topological phases in two-dimensional crystals

Thomas Heine

Leipzig University, Department of Chemistry & Mineralogy, Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, Leipzig, Germany
Jacobs University Bremen, Department of Physics and Earth Science, Bremen, Germany

Since the rise of graphene and other two-dimensional crystals scientists understood that physics in two dimensions is different. There is a large manifold of 2D crystals,[1] many of them showing strong quantum confinement, spin-orbit effects and response to external fields.[2,3] I will present noble metal chalcogenides that exhibit particularly strong quantum confinement. In particular PdS_2 shows a semiconducting phase as monolayer, but a metallic one as bilayer.[4] This property can be exploited in designing a single-metal transistor with negligible contact resistance.[5]
Two-dimensional topological insulators (2DTI), also commonly referred to as quantum spin hall states, have been proposed in 2007, when a HgTe layer was embedded in a CdTe matrix. For layer thickness less than 6.3 nm, the system showed the properties of a 2DTI. Unfortunately, known 2DTI systems have very small bulk band gaps that restricts their application to very low temperature. We are exploring 2D materials that show all characteristics of 2DTI, but have at the same time a large bulk band gap. Here, we concentrate on allotropes of Group 6 transition metal dichalcogenides [6] and on buckled saturated Group 13 and Group 14 phases.[7-9]

References

[1] P. Miro, M. Audiffred, T. Heine, “An Atlas of Two-Dimensional Materials”, *Chem. Soc. Rev.* **2014,** *43,* 6537-6554.

[2] A. Kuc and T. Heine, “The electronic structure calculations of two-dimensional transition metal dichalcogenides in the presence of external electric and magnetic fields”, *Chem. Soc. Rev.* **2015***, 44,* 2603-2614.

[3] T. Heine, “Transition metal chalcogenides: ultrathin inorganic materials with tunable electronic properties”, *Acc. Chem. Res.* **2015***, 48,* 65-72.

[4] P. Miro, M. Ghorbani-Asl, T. Heine, “Two Dimensional Materials Beyond MoS_2: Noble Transition Metal Dichalcogenides”, *Angew. Chem. Intl. Ed. Engl.* **2014***, 53,* 3015–3018.

[5] M. Ghorbani-Asl, A. Kuc, P. Miró, T. Heine, “A single material logical junction based on two-dimensional crystal PdS_2”, *Adv. Materials*, **2015**, accepted for publication.

[6] Y. Ma, L. Kou, X. Li, Y. Dai, S. C. Smith, T. Heine, “Quantum spin Hall effect and topological phase transition in two-dimensional square transition-metal dichalcogenides”, *Phys. Rev. B* **2015***, 92,* 085427.

[7] Y. Ma , Y. Dai , L. Kou , T. Frauenheim, T. Heine, “Robust Two-Dimensional Topological Insulators in Methyl-Functionalized Bismuth, Antimony and Lead Bilayer Films”, *Nano Lett.* **2015***, 15,* 1083–1089.

[8] Y. Ma, X. Li, L. Kou, B. Yan, C. Niu, Y. Dai, T. Heine, “Two-dimensional inversion asymmetric topological insulators in functionalized III-Bi bilayers”, *Phys. Rev. B* **2015***, 91,* 235306.

[9] Y. Ma, L. Kou, A. Du, T. Heine, “Group 14 element based noncentrosymmetric quantum spin Hall insulators with large bulk gap”, *Nano Research* **2015**, 1-9, doi: 10.1007/s12274-015-0842-7.

Optical spectra of atomically thin semiconductors from ab-initio many-body perturbation theory

Thosten Deilmann, Matthias Drueppel, Michael Rohlfing

University of Muenster, Institut for Solid-State Theory, Muenster, Germany

Many-body perturbation theory (MBPT) has emerged as a powerful tool for addressing electronic and optical spectra in low-dimensional systems. We will discuss some recent examples:
(i) The optical spectra of transition-metal dichalcogenides (TMDC) are very sensitive to environmental conditions, like substrate screening, stretching, and bending. Subtle spectral shifts occur and may be used for manipulating optical response by system composition and by mechanical tools.
(ii) TDMC and other low-dimensional semiconductors (e.g., carbon nanotubes, CNT) often exhibit trion states (i.e., charged excitons) that may dominate the luminescence spectrum. We will discuss the evaluation of such three-particle correlation effects within an ab-initio framework and discuss results for CNT.

Electron dynamics in low dimensions: a time- and momentum-resolved view

Isabella Gierz

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When reducing the dimensionality of a material electronic correlations become more and more important with dramatic effects on the electronic properties. Our goal is to engineer the electronic properties of various low-dimensional material systems with light, complementing the more traditional routes of electronic structure control using chemistry, pressure, or magnetic fields. Using the analogy with the Kapitza pendulum, I will show that driven systems are distinct from matter at equilibrium because the interaction with a periodic driving field results in the formation of new effective Hamiltonians with new eigenstates. Famous examples for electronic structure control by periodic driving include light-induced superconductivity in cuprates [1] and K_3C_{60} [2] using resonant excitation of the crystal lattice, as well as the formation of photon-dressed Floquet-Bloch states inducing a topological phase transition in Bi_2Se_3 [3].
I will present our time- and angle-resolved photoemission results on epitaxial monolayer and bilayer graphene for various driving regimes and give a short outlook on recent projects on monolayer transition metal dichalcogenides and hexagonal boron nitride.

References

[1] W. Hu et al., Nature Materials 13, 705 (2014)
[2] M. Mitrano et al., Nature 530, 461 (2016)
[3] Y. H. Wang et al. Science 342, 453 (2013)

Femtosecond exciton and charge dynamics and unusual Stark effect in mono- and few-layer transition metal dichalcogenides

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Recent progress in the exfoliation of layered materials and the nanofabrication of functional structures has revived the interest in two-dimensional materials with properties complementary to graphene, in particular transition metal dichalcogenides (TMDCs). Their potential for electronics has become evident by the realization of a field effect transistor and a logic circuit device based on a single flake of monolayer MoS_2. Despite their high exciton binding energy, mono- and few-layer semiconducting TMDCs show a strong photovoltaic effect and potential for high sensitivity photodetectors. Both these functionalities require efficient charge carrier photogeneration, either via direct excitation of mobile carriers or via exciton dissociation. We use continuous wave photomodulation and femtosecond pump-probe spectroscopy to identify the spectral features of photogenerated charges in an ensemble of few-layer MoS_2 and WS_2 dispersed in a transparent polymer and trace the dynamics of photogeneration and relaxation of both charges and excitons. We find that the primary photoexcitations are excitons which dissociate efficiently with a characteristic time several hundred fs. In WS_2, thanks to the larger separation of the two main excitonics resonances, we can also resolve the carrier trapping after exciton dissociation. While the yield of exciton dissociation into charges is close to unity in the few-layer case, in monolayers it is considerably lower, due to the higher exciton binding energy. We show that the exciton dissociation in monolayer MoS_2 can be enhanced via applying an electric field.

According to our findings, few-layer TMDCs display a behavior which is intermediate between conventional semiconductors on the one hand, and high exciton binding energy materials, such as organic semiconductors, carbon nanotubes, and single-

layer TMDCs on the other. High efficiency photodetectors and photovoltaic elements based on monolayers require additional measures to achieve efficient exciton dissociation, such as a strong built-in field using appropriate electrode materials, engineering a p-n junction, or a heterojunction device. In few-layers, which have the added benefit of absorbing a larger fraction of the incident light, such measures should not be necessary and simpler, more scalable device structures could be used.

To translate electrical into optical signals one uses either the modulation of the refractive index or the absorption of a material by an electric field. Contemporary electroabsorption modulators rely on the quantum confined Stark effect (QCSE), the field-induced red-shift and broadening of the strong excitonic absorption resonances characteristic of low-dimensional semiconductor structures. They require device lengths beyond 100 microns to achieve practical modulation depths of 10 dB. We show an unprecedentedly strong electro-absorption (EA) signal in a monolayer of the two-dimensional semiconductor MoS_2. The EA spectrum is dominated by linewidth broadening of almost 10% at a modulated transverse voltage Vpp = 0.5 V. Contrary to the conventional QCSE, this effect increases linearly with the applied field strength and is due to an increase of the inhomogeneous rather that the homogeneous broadening. The signal magnitude corresponds to a length-specific modulation of up to 75 dB/micron. The extremely compact device design is the only technology to date that can enable on-chip photonic circuit integration.

Electrocatalytic gas capture on 2D nanomaterials

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Electrocatalytic properties of 2D carbon-boron-nitrogen based nanomaterial structures are explored computationally with the application of controllable, highly selective, and reversible CO_2 capture and H_2 storage in mind. Using density functional theory incorporating long range dispersion corrections, we investigated the predicted adsorption behavior of CO_2 on model 2D graphene-like structures with varying charge states. Pyridinic nitrogen incorporation in CNTs is found to induce an increasing CO_2 adsorption energy upon electron injection, leading to a highly selective CO_2 adsorption in comparison with N_2. Similar behaviour has now been found for related 2D C-B-N materials, both conducting and semiconducting in nature. This functionality is intrinsically reversible since capture/release can be controlled by switching the charge carrying state of the system on/off. This phenomenon is verified for a number of different models and theoretical methods, with clear ramifications for the possibility of implementation with a broader class of graphene based membranes.

References

[1] Xin Tan, Liangzhi Kou and Sean C. Smith, “Layered Graphene–Hexagonal Boron Nitride Nanocomposites: An Experimentally Feasible Approach to Charge–Induced Switchable CO2 Capture”, *ChemSusChem*, **8**, 2987-2993 (2015).

[2] Xin Tan, Liangzhi Kou, Hassan A. Tahini, Sean C. Smith, “Charge Modulation in Graphitic Carbon Nitride: An Electrocatalytically Switchable Approach to High-Capacity Hydrogen Storage”, *ChemSusChem*, **8**, 3626-3631 (2015).

[3] Xin Tan, Liangzhi Kou, Hassan A Tahini, Sean C Smith, “Conductive Graphitic Carbon Nitride as an Ideal Material for Electrocatalytically Switchable CO_2 Capture”, *Scientific Reports*, **5**, 17636 (2015).

Electrical control of the optical response of atomically thin semiconductors

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Atomically thin two-dimensional semiconductors are highly attractive for new-generations of (opto-)electronic, photonic and quantum devices. Transition metal dichalcogenides (TMDCs) are of particular interest due to their direct electronic band gap in the monolayer limit, and lack of inversion symmetry that provides direct access to fascinating spin-valley photo-physics. The ability to control the optical and electronic properties of few-layer TMDC crystals is essential for both fundamental physics studies and device applications. In this talk we will present recent studies in which we employ strong (MV/cm) DC-electric fields to control the linear and non-linear optical response of mono- and few-layer 2H-stacked MoS_2 crystals. Few layer crystals are prepared by mechanical exfoliation and embedded within the dielectric region of a Si-SiO_2-TMDC-Al_2O_3-metal photo-capacitor. Such devices provide optical access to the mono and few-layer regions of the TMDC flake while electric fields are applied perpendicular to the basal plane. We observe strong tunability of the A-exciton in emission, with DC Stark shifts up to ~16meV from which we obtain a very low exciton polarisability b= (0.58 ± 0.25) × 10^{-8} Dm V^{-1} consistent with the large binding energy. Interestingly, b is shown to be independent of the thickness of the 2D crystal, indicative of strong localization of both electron and hole wave-functions within each individual layer. Unlike monolayers, bilayer 2H-stacked MoS_2 are inversion symmetric in the absence of applied electric field [1]. Electric fields are shown to result in tuning of the valley optical selection rules and, thereby, the degree of valley polarization can be tuned from η< 20 % to >60% [2]. The local symmetry of the electronic structure is also reflected by the strength of second-harmonic generation (SHG). Hereby, we excite bilayer regions of the MoS_2 crystal at an energy below the A-exciton using ~70 fs duration pulses (E_L=1.24 – 1.47 eV) and detect the signal at $2E_L$. The strength of the SHG signal is found to be strongly dependent on E_L and a pronounced resonance is observed close to the C-peak at $2E_L$=2.75eV. Moreover, the SHG signal is shown to be electrically switchable, increasing by almost two orders of magnitude upon breaking the inversion symmetry with the applied electric field [3]. Finally, if time permits we will present recent data pertaining to localized excitons in hBN-WSe_2-hBN heterostructures. Here, single photon emission is observed from sharp (<0.8meV) emission lines that are clearly located at topological defects on the sample. This observation holds much promise to engineer

the local confinement potential in the TMDC crystal by engineering the dielectric and strain environment. [4]

References

[1] J. Klein and J. Wierzbowski ´, Nano Lett. 2016, 16, 1554−1559
[2] J. Wierzbowski, J. Klein - in course of preparation (2016)
[3] J. Klein and J. Wierzbowski - in course of preparation (2016)
[4] M. Rösner et al, Nano Lett. 2016, 16, 2322-2327

Ultrafast exciton dynamics in 2D TMDC materials

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Transition Metal dichalcogenies have unique optical, electrical and structural properties, resulting in huge binding energies for neutral excitons, biexcitons, and trions. Here, we discuss a detailed spectroscopic investigation of molebdenum ditelluride, and report three different kinds of exciton dynamics, using two-color pump-probe spectroscopy with resonant and nonresonat excitation.

Two-dimensional lateral heterostructures

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Lateral heterostructures are systems where two different 2D materials are joined in the same monolayer plane, forming a 1D interface. We discuss two issues related to topological protection of interface modes, where an inversion of the Dirac mass on either side of the interface generates the non-trivial topology. First, we show how persistent valley and spin currents may be generated along the interface depending on the specific nature of the spin-orbit coupling in the materials. Then we demonstrate that graphenenanoribbons with boron nitride 'cladding' can support topologically protected conducting states, even in the presence of significant crystalline disorder at the interfaces.

Controlling contact resistance in 2D layered materials

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Motivated by metallic graphene, insulating hexagonal-BN monolayer and semiconducting layered transition metal dichalcoginides (LTMDs) have been intensively studied as a new class of transparent and flexible materials, which can be used as essential components of transistors for soft electronics. While large-area graphene is available in a meter-scale, synthesis of large area monolayer h-BN and LTMDs are still a long way to realize. These materials have known to exhibit exotic physical and chemical phenomena which have never been accessed so far with 3D materials. One important issue in 2D materials to use for semiconducting channels is the contact resistance control. Unlike 3D materials like Si where ion implantation is one robust tool to achieve ohmic contact, this method cannot be easily adopted in 2D materials due to facile disintegration of 1D layer. I like to discuss possible methods of reducing contact resistance without deteriorating the contact of 2D materials. This includes phase transition of semiconducting 2H to metallic 1T or 1T phase by light illumination or strain, use of BN as a buffer layer (LTMD/BN/SiO_2) and a passivation layer (h-BN/LTMD/SiO_2).

Tunable optical and electrical properties in 2D semiconductors and their optoelectronic applications

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One of the unique features of atomically thin two-dimensional (2D) materials is strong Coulomb interactions due to the reduced dielectric screening effect; this feature enables the study on unusual excitonic properties in comparison with bulk materials. Optoelectronic applications in 2D transition-metal dichalcogenides (TMDs) are still limited by the weak light absorption, and moreover peak positions and shapes of exciton complexes are sensitively perturbed by varying excitation conditions, inherent from nature of atomically thin layers. Here, we propose a method of selectively amplifying the primary exciton among exciton complexes in TMDs via cyclic re-excitations of cavity-free exciton-coupled plasmon propagations. While TMDs with various bandgaps provide a versatile material library for numerous unexplored physics, artificially stacked van der Waals (vdW) heterojunctions demonstrate ultimate device performances in p-n diodes, photovoltaics, light-emitting diodes, and tunneling field-effect-transistors. A vdW interface quality in HBs, strongly depending on fabrication processes, is a key to understand physical properties and device performances. While heterojunction p-n diodes were well studied via artificial stacking of different TMDs, realizing the homojunction p-n diode is still limited by the absence of a promising strategy for intrinsic carrier type conversion. Here, we demonstrate the vdW homojunction p-n diode having ideal diode characteristics. This was realized by stacking undoped n-$MoSe_2$ on a semiconducting p-$MoSe_2$ synthesized by a traditional elemental doping. The p-type was achieved by Nb substitutional doping during chemical vapor transport synthesis. The fabricated p-n homojunction diode revealed an ideality factor of nearly 1.0. As a consequence of ideal homojunction, a high external quantum efficiency was obtained. Furthermore a clear CMOS inverter operation with a gain of ~0.5 was demonstrated. Our method of simple elemental doping paves a route for realizing not only ideal homojunction diodes but also CMOS logic circuits in a single TMD. Moreover, we demonstrate that a strong vdW coupling constructed by an optimum thermal annealing allows for dominant interlayer-Coulomb interaction and theoretically predicted band renormalization in artificially stacked TMD heterobilayers (HBs). While non-radiative Shockley-Read-Hall (SRH) recombination assisted by interfacial trap sites is predominant in as-fabricated HB diodes, the radiative Langevin process via intricate excitonic emissions are dominant carrier recombination mechanism in post-annealed diodes. Our study suggests a rule to design the vdW interface of devices depending on application purpose and paves a way to construct ideal vdW interface.

Optical properties of 2D semiconductors and hetero-structures

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In this paper we discuss recent advances in our understanding of the optical properties of monolayers of the transition metal dichalcogenide (TMDC) materials, including MoS_2, $MoSe_2$, $MoTe_2$, WS_2, WSe_2. These materials share several unusual characteristics, including a transition from an indirect-gap material in the bulk to a direct-gap, emissive material at monolayer thickness. They also exhibit selectivity to excitation of the degenerate K or K' valley under circularly polarized radiation. In our discussion we will highlight progress in understanding two types of interactions in these materials: the excitonic interactions between charge carriers in one layer and interactions that arise when two monolayer sheets of materials stacked on one another to form a bilayer.

Predicting new 2D materials and exploring the possible applications in energy conversion

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Graphene-based research has progressed quickly following its epoch-making discovery in 2004, but only a handful of realistic applications are available off the shelf due to its inability to act as a semiconductor. Now more research efforts have been devoted to studying other new two-dimensional atomic crystals such as hexagonal boron nitride, metal dichalcogenides and phosphorene etc. Our most recent researches mainly focuses on predicting stability, electronic, mechanical and optical properties in experimentally less-explored two-dimensional materials and exploring possible applications of two-dimensional materials for energy conversion reactions including hydrogen evolution reaction and carbon dioxide conversion. In this presentation, I will share our research progress in relation to the above topics.

Novel 2D interfaces with silicon, graphene, $MoTe_2$ and Ca_2N

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Two-dimensional (2D) interfaces with diverse three-dimensional materials' contact have long been an issue familiar to scientists and engineers. These days, together with 2D materials and emerging 1D edge contact, the 2D interfaces are attracting renewed interests for various applications such as next-generation devices. In particular, polymorph engineering in group 6 TMDs, such as MX_2 with M=(Mo, W) and X=(S, Se, Te), has allowed an intriguing theme in the interface science, a formation of homojunction in a single material.

In this talk, I will briefly review interesting features of 2D interface including graphene [1]. Then, homojunctions between metallic (1T') and semiconducting (2H) $MoTe_2$, generated by two methods (laser irradiation and contacting to low work function material), will be discussed [2]. The synthesis of high quality $MoTe_2$ has been a key for these studies [3]. We demonstrate that our high quality single-crystalline and semimetallic 1T'-$MoTe_2$ exhibits a maximum carrier mobility of 4,000 $cm^2V^{-1}s^{-1}$ and a giant magnetoresistance of 16,000% in a magnetic field of 14 Tesla at 1.8 Kelvin in the bulk form, and the few-layered 1T'-$MoTe_2$ reveals a bandgap of up to 60 meV in its monoclinic form. The small energy difference between 2H and 1T'-$MoTe_2$, resulting in the presence of the two polymorphs, is also used for a novel way of structural phase transition, contact-driven phase change. Extremely low work function of Ca_2N, ~2.3 eV, realizes a large charge transfer that can switch the material's symmetry in a long range of ~100 nm. These interface studies suggest novel contact-based 2D materials design and applications.

References

[1] Heejun Yang et al., Science 336, 1140 (2012).
[2] S. Cho et al., Science 349, 625 (2015).
[3] D. H. Keum et al., Nature Physics 11, 482 (2015).

Photoluminescence and polarization properties of colloidal single-layer TMDC quantum dots

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The presentation will discuss the solution-phase synthesis of size-controlled colloidal WSe_2 single-layer quantum dot(SQD) and the characterization of the nature of absorption and emission affected by the lateral confinement. From single-particle excitation and emission spectroscopy and single-particle polarization anisotropy measurements, we obtained a detailed understanding on the effect of reduction of the lateral dimension on the optical transition energy, vibronic coupling and polarization property of both absorption and emission in WSe_2 SQDs. Based on the findings from colloidal SQDs of WSe_2, similarities and differences between the optical properties of the colloidal SQD and large-size single-layer TMDC sheets will be discussed.

Functional 2D transition metal dichalcogenides: defects, adsorption and magnetism

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In this talk, I will discuss structural, electronic and optical properties of atomic scale defects in 2D transition metal dichalcogenides MX_2, (M = Mo and W; X = S, Se and Te) studied by density functional theory. Various types of defects, e.g., X vacancy, X interstitial, M vacancy, M interstitial, MX and XX double vacancies will be considered regarding their formation energies, defect states and optical properties. Also, it will be discussed how the adsorption characteristics and molecular magnetic properties of functional organometallic molecules are governed by these 2D templates. Some critical features arising from many body treatment of the magnetic centers in the molecules will be discussed.

Multi-scale modelling of devices based on two-dimensional materials

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Two-dimensional materials (2DMs) have only recently entered the nanoelectronic scenario, so that assessing their real performance when exploited for device applications is a complicated task, due to the present embryonic stage of the fabrication process.

In order to provide a comprehensive understanding of the physics at play in 2DMs, multi-scale approach is the only able to provide an accurate insight on the electrical properties and mechanisms in this new class of materials.

In this talk, after presenting the multi-scale approach based on i) the extraction of the main physical quantities at the atomistic level through an ab-initio approach, ii) the definition of the DFT Hamiltonian through a Maximmally Localized Wannier Function basis set and iii) the self-consistent solution of the transport and electrostatics at the device level, we will investigate the performance of some new 2DMs when exploited in thermionic devices.

By means of the developed approach, we will also investigate the performance of vertical and planar heterostructures, which are currently addressed as promising architectures in order to obtain high-performance devices against Industry requirements.

Modulation of electronic structure in low-dimensional transition-metal dichalcogenides

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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. Here, we will present some examples from our recent studies on e.g. noble-metal chalcogenides or Group 14-16 layered systems.

Electronic structure and dynamics at surfaces of 2D TMDCs

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In this contribution some recent results on the ultrafast dynamics in two-dimensional transition-metal dichalcogenides as probed by time- and angle-resolved photoelectron spectroscopy will be presented [1], [2], [3]. In my talk I will focus on the peculiar charge-density-wave states of 1T -$TiSe_2$ and of Rb intercalated 1T -TaS_2.
In detecting the characteristic melting times of electronic order parameters in these materials after pulsed photoexcitation we identify — via systematic temporal discrimination of elementary electronic and structural processes — the dominant interaction responsible for the formation of the ordered low-temperature phases in these materials. Our results show that Rb intercalated 1T -TaS_2 is a Peierls insulator and that the ultrafast response of 1T -$TiSe_2$ is highly suggestive of an excitonic insulator.

References

[1] T. Rohwer, et al., “Collapse of long-range charge order tracked by time-resolved photoemission at high momenta” Nature 471, 490 (2011).

[2] S. Hellmann, et al., „Time-domain classification of charge-density-wave insulators” Nat. Commun. 3, 1069 (2012).

[3] C. Sohrt, et al., „How fast can a Peierls-Mott insulator be melted?” Faraday discussions 171, 243 (2014).

Layered nanostructures – electronic and mechanical properties

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In addition to graphene, 2D transition-metal chalcogenides (e.g., MoS_2 and WS_2), 2D modifications of phosphorus as well as corresponding isoelectronic structures (e.g. SnS) nanostructures are promising materials for applications in electronics and mechanical engineering. Though most of the structures of these materials have an inert surface with a low defect concentration, defects and edge effects can strongly influence the properties of these nanostructured materials. Therefore, a basic understanding of the interplay between electronic and mechanical properties and the influence of defects, edge states and doping is needed. We demonstrate on the basis of atomistic quantum-chemical simulations of selected nanostructures, how the mechanical deformation can vary the electronic properties and other device characteristics of such systems.

Abstracts of Posters

Light-induced topological phase transition in graphene **P01**

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Controlling the electronic properties of a given material system with tailored femtosecond laser pulses is expected to result in a multitude of applications in the field of ultrafast optoelectronics. To date, resonant phonon excitation, where a displacement of the atoms modifies the electronic structure [1,2], or the direct interaction between light and matter resulting in the formation of photon-dressed Floquet-Bloch states [3,4], are the most promising routes to achieve this ambitious goal. The latter is particularly interesting because it is predicted to produce a topological phase transition from a trivial to a topological insulator when driving the sample with circularly polarized light. We investigate the possibility of such a light-driven topological phase transition in epitaxial graphene and its detection with time- and angle-resolved photoemission spectroscopy (tr-ARPES). We will show how, aside from the obvious opening of a band gap at the Dirac point, tr-ARPES is able to detect the predicted non-zero z-component of the pseudospin associated with such a topological phase transition [4].

References

[1] Först et al., Nature Physics 7, 854 (2011)
[2] Subedi et al., Physical Review B 89, 220301(R) (2014)
[3] Wang et al, Science 342, 453 (2013)
[4] Sentef et al., Nature Communications 6, 7047 (2015)

Stacking different two-dimensional materials to fabricate a high mobility transistor

P02

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In recent years, several two-dimensional (2D) semiconducting materials like graphene, MoS_2, WSe_2, silicene, germanene, phosphorene etc. have been produced and intensively studied. Their semiconducting properties allow the development of two-dimensional structures, whose electronic properties can be tuned. By fabricating gate electrodes on the 2D materials, field effect transistors have been demonstrated. In the field of 2D materials, one of the most exciting frontiers is stacking them together which have opened up new opportunities. Different 2D materials are combined in such a way that all their different advantages can be properly utilized to achieve the desired application.

The first series of experiments were carried out with 2D polymers deposited on Si/SiO_2 substrate. A highly sophisticated contacting scheme is developed to contact this material using e-beam lithography while optimizing the desired channel length. In future, the aim will be to fabricate a heterostructure by stacking different 2D materials, whose different properties can complement each other to fabricate a high mobility transistor.

Electrical transport properties of two dimensional CVD molybdenum disulfide (MoS_2)

P03

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Two dimensional materials are attractive for the use in next-generation nanoelectronic devices as compared to one dimensional material because it is relatively easy to fabricate complex structures from them. Recently the layered 2D semiconducting Transition metal dichalcogenides come into the picture and got a place in a wide range of novel applications as well as in basic research. Strikingly, MoS_2 receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.2eV) semiconductor if thinned out to a single atomic layer. The bandgap is an essential property for the tunable 2D nanodevices. We performed the electrical transport measurements at room temperature for the CVD grown MoS_2 on SiO_2/Si substrate. The standard Electron beam lithography (EBL) process was used to pattern the Gold (Au) metal contacts on MoS_2 flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectroscopy techniques respectively which confirm the single layer thickness of CVD MoS_2 triangular flakes on SiO_2/Si substrate. Future work will be based on the low temperature dependence measurements and magneto transport measurements.

In search of controlled single photon emission sites in monolayer transition metal dichalcogenides

P04

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Single photon emission (SPE) from WSe_2 and $MoSe_2$ has recently been demonstrated under both optical and electrical pumping. However, the origin of this emission is still unknown. In this work, we study photoluminescence from exfoliated WSe_2. We find that SPE is observed primarily along the edges of monolayers, including borders with thicker layers. While the properties of the emitted light are consistent with those reported by others, we find that the density and stability of SPE sites depends on the sample preparation method used.

In an attempt to gain insight into the origin of the emission sites, we use off-axis electron holography in the transmission electron microscope and density functional theory calculations to correlate the electron phase measured using electron holography with the bare electrostatic potential in a monolayer WSe_2 crystal. Since the phase can be measured with atomic resolution, we assess the conditions under which point defects (including vacancies and substitutional atoms) can be detected based on their electrostatic potentials using electron holography. We also discuss the possibility of localizing excitons on substitutional atoms (such as, Se in MoS_2) or in lateral heterostructures.

Field-effect doping in transition-metal dichalcogenides from first principles

P05

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We investigate how the large field-effect doping which can be achieved with ionic liquids affects the structural properties, the electronic structure, and the transport properties of few-layers transition-metal dichalcogenides by using DFT. We consider monolayers, bilayers, and trilayers of the H polytype of MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2 and find that, for both electron and hole doping, the electronic structure depends on the number of layers and cannot be described by a rigid band shift. Furthermore, it is important to relax the structure under the asymmetric electric field. Interestingly, while the width of the conducting channel depends on the doping, the number of occupied bands at each given k point is almost uncorrelated with the thickness of the doping-charge distribution. Calculating the inverse Hall coefficient within the constant scattering-time approximation we demonstrate that in some cases the charge determined by Hall-effect measurements can deviate from the real charge by up to 50%. For hole-doped $MoTe_2$ the Hall charge has even the wrong polarity at low temperature. Finally, we report a simple method to extract the scattering time from the experimental conductivity and from the knowledge of the band structure and we show that it is possible to identify the critical doping at which different valleys start to be occupied from the doping dependence of the conductivity.

Gate voltage dependency of Förster resonance energy transfer in graphene - quantum dot photo-detection

P06

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Photo-detectors comprised of a monolayer graphene functionalized by colloidal quantum dots (cQDs) have revealed effective photo detection. Howbeit the detectors are known of being based on a charge or energy transfer, the transfer from the cQDs to graphene is not sufficiently understood. This study examines a graphene field-effect transistor, which is functionalized with CdSe/ZnS core shell cQDs covering it's conductive channel. To investigate energy transfer dynamics in this system, we have measured time-resolved cQD photo-luminescence in dependency of the applied gate voltage. A pronounced increase in the photo-luminescence lifetime has been observed at increasing backgate-voltage, indicating a change of the decay channels. To support our observation, we provide data for a model based on non-radiativeFörster resonance energy transfer as a function of the gating-voltage. The model reveals that by applying an external potential at the backgate, absorption of graphene can be tuned with respect to the photo-luminescence of the cQDs. From this finding a new transfer rate can be calculated.

Origin and manipulation of charge-density-wave state in single-layer $TiSe_2$

P07

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In the last years, 2D materials have gotten the attention of many researchers due to their unique properties and tolerance toward manipulation. In his work we focus our attention on the highly debated transition metal dichalcogenide $TiSe_2$ in its, onolayer phase. For over a decade the transition from the semi-metallic state to the charge density wave state of $TiSe_2$ has been disputed. Here we discuss, based on density functional theory calculations, how this phase transition is a process mediated by the coupling of electrons with the lattice vibrations. As a consequence of this distortion, the monolayer $TiSe_2$ loses its conductive properties. The retrieval of these properties is also studied and presented here as a function of doping.

Electronic structure and ultrafast electron dynamics in epitaxial single layer MoS_2 P08

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Changing the dimensionality of material results in significant modifications of its electronic properties. This is even the case if the parent material already has a layered structure with little interaction between the layers, as in the case of graphene, and the layered transition metal chalcogenides. This poster describes the epitaxial growth of high-quality single-layer (SL) MoS_2 on Au(111) in ultra-high vacuum. Using scanning tunneling microscopy and low energy electron diffraction, the evolution of the growth can be followed from nanoscale SL MoS_2 islands to a continuous MoS_2 layer. An exceptionally good control over the MoS_2coverage is maintained using an approach based on cycles of Mo evaporation and sulfidation to first nucleate the MoS_2 nano-islands and then gradually increase their size. Brief exposure to air is not found to affect the quality of the SL MoS_2. The electronic structure, band gap renormalization and electron dynamics of such layers are investigated by time- and angle-resolved photoemission spectroscopy (ARPES)[1-3]. “Static" ARPES permits the observation of the occupied states, permitting a detailed extraction of the valence band dispersion and the spin-orbit splitting texture in the MoS_2 SL. In the time-dependent experiments, electrons are first excited into the conduction band by a low energy photon and then photoemitted by a high energy photon. This allows us to ascertain a direct quasiparticle band gap of 1.95 eV and to determine an ultrafast (50 fs) extraction of excited free carriers via the metal in contact with the SL MoS_2.

References

[1] J. A. Miwa, S. Ulstrup, S. G. Sørensen, M. Dendzik, AGrubišićČabo, M. Bianchi, J. V. Lauritsen, P. Hofmann, Phys. Rev. Lett. 114, 046802, (2015).

[2] A. GrubišićČabo, J. A. Miwa, S. S. Grønborg, J. M. Riley, J. C. Johannsen, C. Cacho, O. Alexander, R. T. Chapman, E. Springate, M. Grioni, J. V.

Lauritsen, P. D. C. King, P. Hofmann, S. Ulstrup, Nano Letters 15, 5883-5887 (2015).

[3] SørenUlstrup, AntonijaGrubišićČabo, Jill A. Miwa, Jonathon M. Riley, Signe S. Grønborg, Jens C. Johannsen, CephiseCacho, Oliver Alexander, Richard T. Chapman, Emma Springate, Marco Bianchi, MaciejDendzik, Jeppe V. Lauritsen, Phil D. C. King, and Philip Hofmann, ACS Nano in press.

Electrical control of optical processes in atomically thin semiconductors

P09

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We present electrical control of different optical processes in mono- and few-layer 2H stacked MoS_2 crystals driven by an externally applied perpendicular electric field. This is established in a novel lithographically designed Si(n)-SiO_2-STMD-Al_2O_3-metal micro-capacitor device with optical access. By means of electric field dependent low temperature confocal PL we control the direct gap A exciton emission via the quantum confined Stark effect. We observe a layer-independent exciton polarisability which we attribute to the strong localisation of the electron and hole wave function of the A exciton within each individual layer in good accord with reported large exciton binding energies. Selecting the special case of inversion symmetric 2H stacked bilayer MoS_2, we continuously control the valley optical selection rules arising from symmetry considerations, by breaking and restoring the inversion symmetry of the crystal. We demonstrate strong tunability of the degree of circular polarisation of the emission from η = 20% up to 58%. Based on the same control parameter, intense tunability of second-harmonic generation in naturally inversion symmetric 2H stacked bilayer MoS_2 is demonstrated. We excite bilayer MoS_2 crystals with pulses of ~70 fs within a spectral window of 840 – 1000 nm (1.24 – 1.47 eV) and observe a significant tunability throughout the probed region with a ~60 fold conversion amplification at its optimum.
Our results demonstrate the potential for electric field controlled devices for control of excitonic emission energies, emergent valley photo-physics and efficient electrically driven broadband frequency doubling by external control of the symmetry properties of 2H bilayer MoS_2.

Room temperature quantum spin Hall states in two-dimensional crystals composed of pentagonal rings and their quantum wells

P10

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Quantum spin Hall (QSH) insulators are a peculiar phase of matter exhibiting excellent quantum transport properties with potential applications in lower-power-consuming electronic devices. Currently, among all predicted or synthesized QSH insulators, square and hexagonal atomic rings are the dominant structural motifs, and QSH insulators composed of pentagonal rings have not yet been reported. Here, based on first-principles calculations, we predict a family of large-gap QSH insulators in SnX_2 (X=S, Se, or Te) two-dimensional (2D) crystals by the direct calculation of Z2 topological invariants and edge states. Remarkably, in contrast to all known QSH insulators, the QSH insulators predicted here are composed entirely of pentagonal rings. Moreover, these systems can produce sizeable nontrivial gaps ranging from 121 to 224 meV, which is sufficiently large for practical applications at room temperature. Additionally, we propose a quantum well by sandwiching an $SnTe_2$ 2D crystal between two $BiOBiS_2$ sheets and reveal that the considered 2D crystal remains topologically nontrivial with a sizeable gap. This finding demonstrates the robustness of its band topology against the effect of the substrate and provides a viable method for further experimental studies.

Magneto-optical investigation of exciton fine structure in monolayer tungsten diselenide

P11

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The transition metal dichalcogenides (MoS_2, $MoSe_2$, WS_2, WSe_2,..) are quasi two dimensional layered materials with a band gap in the visible/near infrared. A monolayer is composed of a single layer of transition metal embedded between two atomic layers of chalcogenides atoms in a trigonal prismatic structure. The weak interlayer coupling nevertheless completely modifies the band structure. Bulk crystals are indirect semiconductors with extremely weak phonon assisted photoluminescence emission. Monolayer dichalcogenides on the other hand have a direct band gap located in two degenerate valleys (K) at the corner of hexagonal Brillouin zone and the PL emission is enhanced by many orders of magnitude compared to bulk crystals.

In this work we compare the optical response of different monolayer WSe_2 samples in the presence of high magnetic fields. We show that in monolayer WSe_2 the exciton exhibits a splitting which originates from both moderate strain and lifting of the valley degeneracy in a magnetic field.

Morphology and electronic structure of single-layer TaS_2 **P12**

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Single-layer TaS_2 is epitaxially grown on Au(111) substrates. The resulting two-dimensional crystals adopt the 1H polymorph. The electronic structure is determined by angle-resolved photoemission spectroscopy and found to be in excellent agreement with density functional theory calculations for the 1H polymorph. Neither superconducting nor charge density wave states are observed at temperatures down to 4.7 K; the possibility that charge density wave states might be suppressed due to slight doping is considered.

Exciton dynamics in two-dimensional materials with strong spin-orbit interaction: $MoSe_2$ versus WSe_2

P13

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Monolayers of semiconducting transition metal dichalcogenides (TMDCs) such as MoS_2, WS_2, $MoSe_2$ and WSe_2 have attracted considerable attention following the discovery of the indirect-to-direct bandgap transition from bulk to monolayer material and the coupling of spin and valley degrees of freedom in atomically thin layers. An important characteristic of these compounds is the strong spin-orbit interaction, which leads to a splitting between dark and bright exciton sub-bands. The spin-orbit splitting has different signs for $MoSe_2$ and WSe_2 and is expected to influence the carrier dynamics as well as the resulting photoluminescence (PL) yield. A detailed understanding of dark and bright exciton dynamics and non-radiative processes is important for light emitting applications as has been demonstrated in other systems such as phosphorescent organic light emitting diodes.

We measure time-integrated and time-resolved PL in monolayers of WSe_2 and $MoSe_2$ in a wide range of temperatures from 10 to 300K and gain insights into the exciton and trion dynamics.

Our study reveals similar carrier dynamics for both materials, whereas pronounced differences have been observed for the overall PL intensities. In $MoSe_2$, the PL decreases strongly with temperature accompanied by a decrease of the exciton decay time up to a temperature of about 130K. For WSe_2 the PL intensity and exciton decay time both increase with temperature above 200K.

We attribute the increase of the WSe_2 PL intensity to the thermally activated population of the higher energy bright exciton sub-band. In $MoSe_2$, where the bright exciton sub-band is the lowest energy state, the observed behavior indicates high efficiency of non-radiative processes, which appear to be slow in WSe_2. For high temperatures the rise of the decay time in both materials can be attributed to a light cone effect, which has been observed recently in MoS_2.

Multiferroic two-dimensional materials **P14**

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The relation between unusual Mexican-hat band dispersion, ferromagnetism and ferroelasticity is investigated using a combination of analytical, first-principles and phenomenological methods. The class of material with Mexican-hat band edge is studied using the α-SnO monolayer as a prototype. Such band edge causes a van Hove singularity diverging with $\frac{1}{\sqrt{E}}$ and a charge doping in these bands can leads to time-reversal symmetry breaking. Herein, we show that a material with Mexican-hat band dispersion, α-SnO, can be ferroelastic or paraelastic depending on the number of layers. Also, an unexpected multiferroic phase is obtained in a range of hole density for which the material presents ferromagnetism and ferroelasticity simultaneously.

Restacking effects on the elctronic properties of bilayer 1T phase of MoS_2

P15

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In this study, we have employed the density functional theory (DFT) to investigate the Van der Waals (vdW) interlayer spacing between the two layers of bilayer 1T phase of MoS_2 (1T-MoS_2) and the superstructures derived from bonding associations of metal atoms of restacked 1T-MoS_2 [1,2]. We observed that Mo atoms form clusters and localized zigzag chain clusters on the two layers of bilayer system after geometric optimization. The vdW interlayer distance (equilibrium interlayer distance d_o) has been optimized using DFT by computing the total energy as a function of the interlayer distance d, which was varied between 5A and 7A while keeping the in-plane lattice constant fixed at the bulk value. In order to evaluate the binding energy in 1T-MoS_2 bilayer system energy difference has been evaluated between the total energy values at equilibrium distance d_o and at d=7A, which gives a value for the limit of infinite layer distance for 1T-MoS_2. Recently experimental reseaches have focused on the exfoliation of layered materials to two dimensional nanosheets and then restacking them to form electrodes [3-8]. We observed that metallic 1T-MoS_2 can intercalate ions efficiently which shows that 1T phase of MoS_2 can be used as supercapacitor electrode materials.

References

[1] J. Am. Chem. Soc. 121, 638-643, 1999
[2] J. Am. Chem. Soc. 121, 11720-11732, 1999
[3] Nano Lett. 8, 3498-3502, 2008
[4] Science 341, 1502-1505, 2013
[5] Science 332, 1537-1541, 2011
[6] J. Am. Chem. Soc. 133, 17832-17838, 2011
[7] Chem Commun. 46, 1106, 2010
[8] Nature Nanotechnology 10, 313-318, 2015

Isingspintronics in transition-metal dichalcognides

P16

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Based on exact diagonalization method, the ground state and the spin lifetime of magnetic adatoms with d9 electronic configuration on monolayer transition-metal dichalcognides (TMDCs) are calculated under a specific crystal field. Results show that the system exhibits a large Ising-type magnetic anisotropy and the spin lifetime sensitively depends on the type and concentration of carriers, suggesting an electrical approach to manipulate the spin state of magnetic adatoms on TMDCs. Further, our ab initio calculations suggest that this Ising-type spintronics can be realized in Co, Rh, or Iradatoms on MoS_2.

Long-lived quantum emitters in hBN/WSe_2 van-der-Waals heterostructures

P17

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We present the formation of single photon emitters in 2D hBN/WSe_2/hBN van-der-Waals (vdW) heterostructures. By means of viscoelastic stamping [1], we encapsulate monolayer WSe_2 using multi-layer hBN crystals as substrate and capping materials, respectively, symmetrizing the dielectric environment of the semiconducting crystal. Upon encapsulating the WSe_2 in hBN, we observe a linewidth of ~4 meV for the X^0 and X^- transitions, a reduction of 50% as compared to WSe_2 placed directly on Si/SiO_2 substrates. This effect has been interpreted as arising from suppressed non-radiative decay channels due to the hBN encapsulation of the semiconductor [2]. Using low excitation power densities ($P < 2$ W/cm²), we observe localized sharp emission lines (FWHM < 1 meV) ~100 meV below the exciton PL energies. Second-order photon correlation measurements demonstrate anti-bunching light behaviour. Time-resolved PL measurements reveal a 10-fold prolonged lifetime of the localized emitters $t \approx 25$ ns, as compared to other recent works [3-4]. The spectral jitter of the sharp spectral lines exhibits a 1/f frequency behaviour, possibly due to a thermally fluctuating charge environment. In polarization-resolved experiments, we observe a significant fine structure splitting of single emission lines ranging from 0.5 meV to 1 meV. Employing a ZrO_2 solid immersion lens (SIL) as a substrate and, thus, enhancing the spatial resolution by a factor of ~5, we measure the upper bound of the spatial extend of the localized emitters in WSe_2 of 250 nm. Our results demonstrate the potential of employing hBN as a high quality substrate for optimized optical properties of delocalized and localized emission of excitons in WSe_2.

References

[1] Castellanos-Gomez, A. et al. Deterministic transfer of two-dimensional materials by all-dry viscoelastic stamping. 2D Mater. 1, 011002 (2014).

[2] Tonndorf, P. et al. Single-photon emission from localized excitons in an atomically thin semiconductor. Optica 2, 347 (2015).

[3] Koperski, M. et al. Single photon emitters in exfoliated WSe2 structures. Nat. Nanotechnol. 10, 503–506 (2015).

[4] Srivastava, A. et al. Optically active quantum dots in monolayer WSe2. Nat. Nanotechnol. 10, 491–496 (2015).

In situ off-axis electron holography of electrically biased two-dimensional transition metal dichalcogenides

P18

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Transition metal dichalcogenides (TMDs), such as MoS_2 and WSe_2, have attracted much attention in recent years due to their enormous potential for applications in nanoelectronic devices. However, the electrical properties of mono- or few-layer TMDs can be influenced strongly by the presence of contamination and defects, as well as by their interfaces to three-dimensional metal contacts.
Off-axis electron holography allows the projected electrostatic potential of a nanoscale specimen to be measured in the transmission electron microscope. The technique can therefore be used to correlate the structural and compositional properties of TMDs with their electronic properties by performing in situ electrical biasing experiments. Here, we present first results and discuss the challenges and prospects of performing electron holography on individual electrically biased MoS_2 devices. The electrical contacts are patterned using electron beam lithography on a SiN membrane. In order to provide a vacuum reference wave for off-axis electron holography, the MoS_2 flakes are partly suspended over holes in the SiN membrane.

Ab initio studies of dynamical properties of chosen group VI-B transition metal dichalcogenides systems

P19

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Recently, group-VIB transition metal dichalcogenides (TMDCs) attract significant interest due to their extraordinary and tunable electronic and optical properties. Their quasi two-dimensional character leads to the anisotropy of their physical properties, which has various technological applications. Moreover, the mixed layered crystals allow for continuous tuning of the optical bandgap, rendering the TMDCs alloys the appealing materials for applications in electronic and optoelectronic devices. Hence, an experimental characterization and theoretical analysis of the properties of mixed crystals is of fundamental importance. This work is focused on the phonon properties of chosen TMDC systems, especially the influence of composition variations in mixed crystals.

We study from first principles (DFT) dynamical properties of several MX_2 bulk crystals and thin films (M=Mo, W, Re; X=S, Se, Te). Dynamical properties of $MoS_xSe_{(1-x)}$ alloys are investigated within a supercell model for different compositions x. The calculated phonon dispersions and densities of states reproduce well the measured Raman spectra.

We are able to explain the evolution of Raman modes by analysing the projected phonon density of states at Γ point of reciprocal space. Additionally, we develop a phonon dispersion unfolding technique which simplifies the crowded supercell phonon dispersions and allows for a direct comparison with experimental data.

Light matter interaction, exciton-phonon coupling and optoelectronic properties in TMDCs

P20

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Transition metal dichalcogenides such as MoS_2 are of current interest for optoelectronic, sensing and energy harvesting application, but also for studying fundamental aspects of light-matter interaction in strictly two-dimensional semiconductors. We access the complex dielectric function of MoS_2 flakes with a high lateral resolution by spectroscopic imaging ellipsometry [1]. The significant excitonic transitions close to the band gap as well as at high energies are only well observed in the in-plane component of the dielectric tensor and display a fascinating fine-structure. The importance of excitonic effects emerge also in resonant Raman spectroscopy, where unexpected polarization dependence point towards strong exciton-phonon coupling in MoS_2.
We further utilize non-resonant Raman spectroscopy on MoS_2 to study the effect of physisorbed environmental molecules [2] and to investigate the photo-stability in water [3]. The observed photo-catalytic stability highlights the potential of MoS_2 monolayers as high efficient photo-catalyst for solar driven water-splitting applications. In the scope of photo-catalysis and in general for optoelectronic application, the dissociation dynamics of photo-excited e-h pairs is of great relevance. Therefore, the dynamic of photo-excited charge carriers on a picosecond time scale is monitored by photocurrent measurements utilizing a recently developed pump-probe spectroscopy technique based on coplanar striplines [4-6]. These investigations provide access to the mechanisms for photocurrent generation, charge dissociation and the related charge transport dynamics.
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References:

[1] S. Funke et al., arXiv:1603.06644 (2016).
[2] B. Miller, et al., Appl. Phys. Lett. 106, 122103 (2015).
[3] E. Parzinger et al., ACS Nano, 9(11), 11302 - 11309 (2015).
[4] L. Prechtel, et al. Nature Communications 3, 646 (2012).
[5] A. Brenneis et al. Nature Nanotechnology 10, 135 (2015).
[6] C. Kastl et al. Nature Communications 6, 6617 (2015).

Two dimensional rectangular tantalum carbide halides TaCX (X = Cl, Br, I): novel large-gap quantum spin Hall insulators

P21

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Quantum spin Hall (QSH) insulates exist in special two-dimensional (2D) semiconductors, possessing the quantized spin Hall conductance that are topologically protected from back scattering. However, known QSH materials (e.g. HgTe/CdTe and InAs/GaSb quantum wells) exhibit very small energy gap and only work at low temperature, hindering their applications for room temperature devices. Moreover, most of predicted or synthesized QSH insulators are confined to main-group-elements-based compounds, and the number of transition metal-based QSH insulators is still extremely scarce. Based on the first-principles calculations, we predict a novel family of QSH insulators in 2D tantalum carbide halides TaCX (X = Cl, Br, and I) with unique rectangular lattice and large direct energy gaps (>0.23 eV). The mechanism for 2D QSH effect originates from an intrinsic d−d band inversion, different from that inconventional QSH systems (such as s−p or p−p band inversion). Further, stain and intrinsic electric field can be used to tune the electronic structure and enhance the energy gap. TaCX nano ribbon, which has the single-Dirac-cone edge states crossing the bulk band gap, exhibits a linear dispersion with a high Fermi velocity comparable to that of graphene. These 2D materials with considerable nontrivial gaps promise great application potential in the new generation of dissipation less electronics and spintronics.

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