O 53: 2D Materials II: Transition Metal Dichalcogenides

Time: Wednesday 10:30–13:15 Location: H16

O 53.1 Wed 10:30 H16

Ultrafast Photo-induced Phase Transition in 2D MoTe2 — •Bo Peng — TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — Key Laboratory of Micro and Nano Photonic Structures (MOE), Department of Optical Science and Engineering, Fudan University, Shanghai 200433, China

For phase transition in 2D solids, lots of amazing physical phenomena remain to be understood as compared with the intensively investigated 3D one. A central topic is the nature of photo-induced phase transition in monolayer MoTe2. Using first-principles calculations, we pinpoint that the phase transition from 2H to 1T' phase is induced by purely electronic excitations within several hundred femtoseconds, far shorter than conventional structural phase transition. Such excitation initially changes the chemical bonding. As laser excitation energy is increased to 2 eV, the lattice vibrational modes are softened, leading to symmetry breaking displacements and generating the intermediate structures along the phase transition pathway. The distortions are strongly dependent on laser energy, enabling controllable phase transformation by varying laser wavelength. Our results identify an ultra-rapid and controllable phase transformation mechanism in monolayer MoTe2, opening a new door for precise control of ultra-fast phase transition in low-dimensional systems by tuning laser energy.

O 53.2 Wed 10:45 H16

Angle, spin and time-resolved photoemission spectroscopy on WSe2 — •zakariae el youbi[1,2,4], jakub schüsser[1,3,4], mauro fanciulli[1,4], waly ndiaye[1,4], olivier heckmann[1,4], marie-christine richter[1,4], cephise cacho[2], and karol hricovini[1,4] — [1]LPMS, UCP, Cergy, France — [2]Diamond Light Source, Harwell Campus, Didcot OX11 0DE, UK — [3]Univ. of West Bohemia, Plzeň, Czech Republic — [4]LIDYL-UMR 9222 CEA-CNRS

Tunable bandgap, high specific surface area, fabrication of van der Waals heterojunctions and other specific electronic properties make Transition Metal Dichalcogenides (TMDCs) very promising for the applications in photovoltaics and optoelectronics. In particular WSe2 which is of interest for valleytronic and spintronic device concepts. Here we report the characterization of cleaved WSe2 samples by angle resolved photoemission spectroscopy (ARPES). We measured the band structure of the valence band along Γ - K and Γ - M directions with Helium I and Helium II radiation and as well with ultrashort ($<$ 20 fs) HHG laserlight. Ultrafast dynamics by pump-probe experiments (trARPES) and spin analysis in combination with circular polarised excitation will be discussed.

O 53.3 Wed 11:00 H16

Hyperbolic light dispersion in MoTe2 from many-body perturbation theory: impact of dimensionality — •Saeideh Edalati Boostan, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Among the transition-metal dichalcogenides, MoTe2 shows only a moderate decrease of photolouminescence intensity with increasing number of layers, which makes it an excellent candidate for opto-electronic applications [1]. Therefore, it is essential to gain insight into the response of this material to electro-magnetic radiation with respect to the number of layers. We investigate the electronic and optical properties of MoTe2, considering a monolayer, a bilayer, and its bulk form. Our study is based on many-body perturbation theory including GW and the Bethe-Salpeter equation (BSE), as implemented in the exciting code [2]. Our BSE results reveal that MoTe2 is a natural type-II hyperbolic material in a window of a few eV between the visible and the ultraviolet (UV) region. We emphasize the importance of including many-body effects for a proper quantitative description of this phenomenon. Going from the monolayer to the bulk, the energy window of hyperbolicity is red-shifted by several tenths of an eV. These findings disclose new perspectives for this material in view of applications in plasmonics and nano-imaging.

[1] I. G. Lezama, et al., Nano Lett. 15 (2015) 2336.
[2] A. Gulans, et al., JPCM 26, 36 (2014).

O 53.4 Wed 11:15 H16

Ultrafast charge transfer in epitaxial WS_2/graphene heterostructures — •Razvan Krause[1], Sven Aeschlimann[1], Antonio Rossi[2,3], Mariana Chavez-Cervantes[1], Stiven Forti[2], Filippo Fabbri[2,4], Camilla Coletti[2,4], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany — [2]Center for Nanotechnology Innovation at NEST, Italian Institute of Technology, Pisa, Italy — [3]NEST, Istituto Nanoscienze, CNR and Scuola Normale Superiore, Pisa, Italy — [4]Graphene Labs, Istituto Italiano di Tecnologia, Genova, Italy

We use time- and angle-resolved photoemission spectroscopy (tr-ARPES) to investigate ultrafast charge transfer in an epitaxial heterostructure made of monolayer WS_2, a direct gap semiconductor with strong spin-orbit coupling, and graphene, a semimetal hosting massless carriers with extremely high mobility. We find that, after photoexcitation at resonance to the exciton in WS_2, the photo-excited holes rapidly transfer into the graphene layer while the photo-excited electrons remain in the WS_2 layer. The resulting charge transfer state is found to have a lifetime of ˜1ps [1]. While the overall dynamics can be understood in terms of the relative alignment of the WS_2 and graphene band structures [2], the microscopic mechanism of the observed ultrafast charge transfer remains elusive. We present tr-ARPES data for different pump fluences and pump wavelengths and discuss our results in the context of recent theoretical work on the subject [3,4].

O 53.5 Wed 11:30 H16

Exciton propagation in TMDC monolayers at room temperature — •Marvin Kulig[1], Jonas Zipfel[1], Philipp Nagler[1], Sofia Blanter[1], Jonas Ziegler[1], Christian Schüller[1], Tobias Korn[1], Nicola Paradiso[1], Misha Glazov[2], and Alexey Chernikov[1] — [1]Department of Physics, University of Regensburg — [2]Ioffe Institute, Saint Petersburg, Russian Federation

In our work, we examine two dimensional exciton transport of several TMDC materials by directly monitoring the excitonic emission of the optically excited system through spatially- and time-resolved photoluminescence. In order to suppress effects from the silicon oxide substrate roughness, we additionally produce samples encapsulated between thin layers of hexagonal boron nitride. Depending on the injected exciton density, we observe highly nonlinear behavior with characteristic, qualitative changes in the spatial profiles, which results in an increase of the measured effective diffusion coefficient of up to two orders of magnitude. Solving the diffusion equation in consideration of Auger recombination provides the main interpretation and a physical basis of the observed phenomena. For the encapsulated monolayers, Auger recombination is highly suppressed, while the linear diffusion coefficient is more than one order of magnitude larger than for the as-exfoliated, non-encapsulated monolayers.

O 53.6 Wed 11:45 H16

Spatial extent of the excited exciton states in WS2 monolayers from diamagnetic shifts — •Jonas Zipfel[1], Johannes Holler[1], Anatolie A. Mitioglu[2], Mairana V. Ballotin[2], Philipp Nagler[1], Andreas V. Stier[3], Takashi Taniguchi[4], Kenji Watanabe[4], Scott A. Crooker[3], Peter C. M. Christianen[2], Tobias Korn[1], and Alexey Chernikov[1] — [1]Department of Physics, University of Regensburg D-93053, Germany — [2]High Filed Magnet Laboratory (HFML -EMFL), Radboud University, 6525 ED Nijmegen, The Netherlands — [3]National High Magnetic Field Laboratory, Los Alamos, New Mexcio 87545, USA — [4]National Institute for Materials Science, Tsukuba, Ibaraki 305-004, Japan

Owing to strong Coulomb interactions, the properties of monolayer TMDCs are governed by the formation of tightly bound electron-hole pairs, with binding energies as high as 0.5 eV. This motivates questions of the appropriate description of these exciton states and in particular, their spatial extent. We use magneto-optical reflectance spectroscopy in fields up to 29T to detect energy shifts of exciton ground and excited state resonances in encapsulated WS2 monolayers. These characteristic shifts arise both due to the valley Zeeman and diamagnetic effects. We find similar Zeeman shifts for ground and excited states. An analysis of the diamagnetic shifts allows us to draw direct conclusions on the spatial extent of the exciton states. Exciton radii of about 2nm for the ground and, more importantly, up to 5-8nm for the excited state

are obtained, further confirming the applicability of a Wannier-Mott like description of excitons in monolayer semiconductors.

O 53.7 Wed 12:00 H16

Impact of excitons in transition metal dichalcogenides on time-resolved ARPES — •Dominik Christiansen[1], Malte Selig[1], Ermin Malic[2], and Andreas Knorr[1] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden

Time- and angle resolved photoemission spectroscopy (trARPES) allows to study the dynamics of electronic excitations exploiting the photoelectric effect: A VIS pump pulse creates a non-equilibrium electron occupation dynamics detected by a time delayed XUV probe pulse, examplary performed in ultrathin transition metal dichalcogenides (TMDs) [1]. However, these materials exhibit strongly bound excitons, a complex quasi-particle band structure and their interplay dominate the trARPES spectrum [2].

Here, we develope an excitonic theory of time- and angle resolved photoemission spectroscopy investigating the exciton dynamics at different high symmetry points of the Brillouin zone [3].

[1] R. Bertoni et. al., Phys. Rev. Lett. 117, 277201 (2016)
[2] A. Steinhoff et. al., Nat. Commun. 8, 1166 (2017)
[3] M. Selig et. al., 2D Mater. 5, 035017 (2018)

O 53.8 Wed 12:15 H16

Tensor-Networks for calculating biexcitons in single layered materials — Sandra C. Kuhn and •Marten Richter — Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Germany

The calculation of biexciton states is a numerical very demanding problem due to the high number of involved carriers (two electron-hole pairs). In addition, the rich structure of the Brioullin Zone in two dimensional single layer TMDCs requests an accurate grid on the full Brioullin zone. We show, that a combination of tensor networks with logical circuits lifts this numerical burden and reduce the biexciton problem from a super computer to a workstation problem. Results for excitons and biexcitons in MoS_2 are discussed. Furthermore the method shows potential for future application including quantum dynamics of electron-hole complexes.

[1] S. Kuhn, M. Richter arXiv:1807.09036

O 53.9 Wed 12:30 H16

A many-body view on electronic excitations in TMDCs — •Philipp Marauhn, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Semiconducting transition metal dichalcogenides (TMDCs) have remarkable physical properties. Their two-dimensional nature in the monolayer limit leads to high exciton binding energies of several hundreds of milli-electronvolt. In this talk we discuss effects on the excited states that arise when stacking monolayers into multilayer or bulk systems.

To investigate electronic excitations in TMDCs we employ ab-initio many-body perturbation theory. Notably we solve the Bethe-Salpeter equation on the basis of a preceding LDA+*GdW* calculation, which is a simplified version of the *GW* method. Our results show that screening is a crucial ingredient when describing the optical spectra of TMDCs. Stacking layers on top of each other results in an enhanced screening environment shifting exciton resonances towards lower energy. This redshift is in agreement with experimental differential reflectance measurements [1]. Another effect of stacking is the admixture of pure intralayer excitons with charge transfer configurations.

[1] Y. Niu et al., Nanomaterials, **8**, 725 (2018)

O 53.10 Wed 12:45 H16

De-excitation dynamics in 2D MoS_2 with defects — •Raquel Esteban-Puyuelo[1], Alexey Akimov[2], and Biplab Sanyal[1] — [1]Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Box-516, SE 75120, Sweden — [2]Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, New York 14260-3000, USA

Single layer transition metal dichalcogenides (TMDs), e.g., MoS_2 can be considered as graphene analogues with interesting electronic and optical properties for practical applications, mainly due to their semiconductor nature. Understanding its fundamental properties such as the mechanism of photoinduced de-excitation dynamics is crucial so that TMDs can make the transition from research labs to modern technologies. We have investigated the role of point defects in modifying the direct recombination time of monolayer MoS_2 using time-dependent ab initio non-adiabatic molecular dynamics simulations. We determine which defects would undermine the performance of realistic devices built with this material, as well as the mechanisms behind this effect.

O 53.11 Wed 13:00 H16

Exciton landscape of mono- and bilayer transition metal dichalcogenides — •Thorsten Deilmann and Kristian Sommer Thygesen — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Monolayers and bilayers of transition metal dichalcogenides are intensively studied, in particular due to their rich opto-electronic properties. Until now the main focus has been the investigation of (bright) excitons with zero momentum. In this study we employ *ab initio* many-body perturbation theory within the *GW*/BSE approximation to describe the entire q-resolved exciton band structure for mono- and bilayers of the MX_2 (M = Mo, W and X = Se, S) TMDCs.

We find that excitonic effects strongly influence the exciton band structure. However, energy differences between extrema with varied exciton momenta can be described fairly well already within DFT.