MA 40: Graphene-like materials: Silicene, MoS_2 and relatives (with DY/DS/HL/O/TT)

Time: Thursday 10:00–12:30 Location: POT 081

MA 40.1 Thu 10:00 POT 081

Many-body effects in 2D hexagonal semimetals and semiconductors — •Tineke Stroucken, Johanna Grönqvist, and Stephan W. Koch — Department of Physics and Material Sciences Center, Philipps University Marburg, Renthof 5, D-35032 Marburg, Germany

Recently, a variety of graphene-analogues materials like h-BN, silicene or transition-metal dichalcogenides have been fabricated. Similar to graphene, these novel material systems display exciting new physical properties, distinct from their bulk counterparts.

Owing to the symmetry of the hexagonal lattice, band edge carriers are described by massive Dirac Fermions. Typically, the Fermi-velocity is in the range of $c/300$ or below. This yields effective fine structure constants $\alpha = e^2/\epsilon\hbar v_F \gtrsim 2/\epsilon$, implying prominent Coulomb interaction and relativistic effects. Particularly, $\alpha \gtrsim 1$ indicates an excitonic instability of the noninteracting ground state.

In this presentation, we discuss conditions for strong Coulomb coupling in 2D hexagonal crystals and identify experimentally observable signatures signaling an excitonic ground state. To this end, the gap equations are solved self consistently with the polarization function, which depends on the interacting band structure.

[1] T. Stroucken *et al.*, Phys. Rev. B 84, 205445 (2011)
[2] J. H. Grönqvist *et al.*, EPJ B 85, 12 (2012)
[3] T. Stroucken *et al.*, Phys. Rev. B. 87, 245428(2013)
[4] T. Stroucken *et al.*, Appl. Phys. Lett. 103, 163103 (2013)

MA 40.2 Thu 10:15 POT 081

Single and Multi-Layer Silicene: Growth, Properties and Perspectives — •Patrick Vogt[1], Thomas Bruhn[1], Andrea Resta[2], Paola De Padova[3], and Guy Le Lay[2] — [1]Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Aix-Marseille University, CNRS- PIIM UMR 7345, F-13397 Marseille Cedex 20, France — [3]Instituto di Struttura della Materia, Consiglio Nazionale delle Ricerche -ISM, via Fosso del Cavaliere, 00133 Roma, Italy

Silicene, a new silicon allotrope with a graphene-like honeycomb structure, has recently attracted considerable interest, because its topology confers to it the same remarkable electronic properties as those of graphene, with the potential advantage of being easily integrated in current Si-based nano/micro-electronics offering novel technological applications.

We will discuss the epitaxial formation of single layer silicene on Ag substrates and its structural and electronic properties [1-2]. Based on these results we will look at the growth of silicene multi-layers which can be explained by stacking of single silicene sheets [3-4]. Different experimental techniques are used to investigate atomic structure and electronic properties of this layered system and to discuss its similarities to graphite.

1) Vogt, P. et al., Phys. Rev. Lett. 108, 155501 (2012).
2) Avila, J. et al., J. Phys.: Condens. Matter 25, 262001 (2013).
3) De Padova, P.; Vogt, et al. Appl. Phys. Lett. 102, 163106 (2013).
4) Resta, A. et al., Sci. Rep. 3, 2399 (2013).

MA 40.3 Thu 10:30 POT 081

Optical and vibrational properties of MoS2 — •Ludger Wirtz[1], Alejandro Molina-Sanchez[1], and Kerstin Hummer[2] — [1]Physics and Materials Science Research Unit, University of Luxembourg — [2]Faculty of Physics, University of Vienna, Austria

Monolayer MoS2 is currently receiving a lot of attention as a potential alternative to graphene. Its band gap of about 2eV (depending on the dielectric environment) makes it a suitable candidate for thin-film electronics. The optical and vibrational properties of mono-layer, few-layer, and bulk are seemingly straightforward to calculate. Nevertheless some surprises occur: the phonon dispersion displays an anomalous Davydov splitting and the optical absorption spectra display a rich structure of excitonic peaks in the band-gap and in the continuum of interband transitions. We give a short review of the state-of-the art and discuss recent advances in the understanding of the influence of the substrate on the vibrations and electronic excitations.

MA 40.4 Thu 10:45 POT 081

Carrier- and valley dynamics of singlelayer MoS_2 — •Gerd Plechinger[1], John Mann[2], Christian Schüller[1], Ludwig Bartels[2], and Tobias Korn[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Chemistry, Physics, and Materials Science and Engineering, University of California, CA 92521 Riverside, USA

Consisting of an only 0.7 nm thin S-Mo-S sheet and offering a direct bandgap at the K-points in the Brillouin zone, singlelayer MoS_2 represents a promising semiconductor material for flexible and transparent optoelectronic applications. By means of chemical vapor deposition (CVD), large-area films (several mm^2) of singlelayer MoS_2 can be produced. These were characterised by photoluminescence and Raman spectroscopy. In order to investigate the carrier dynamics, we performed pump-probe measurements in the spectral range of the optical transitions in singelayer MoS_2. Helicity-resolved PL measurements have demonstrated an efficient valley polarisation of the K^+ or K^- valley at near-resonant excitation. We probe these valley dynamics with Kerr spectroscopy and find a biexponential decay of the valley polarisation with decay times of a few tens of ps and a few hundreds of ps at low temperatures.

Coffee break (15 min.)

MA 40.5 Thu 11:15 POT 081

Photocurrent studies on semiconducting MoS2 — Marina Hoheneder, •Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching

The current interest in transition metal dichalcogenides is stimulated by their peculiar electrical and optoelectrical properties and their potential for novel device applications. We investigate the semiconductor MoS2, which shows a crossover from an indirect to a direct bandgap semiconductor by thinning it down to a monolayer. We prepare MoS2 samples through micromechanical exfoliation and characterize the thin flakes with Raman spectroscopy. We further study photocurrent generation of single and few layer MoS2 in dependence of wavelength and power of the exciting light. We gratefully acknowledge financial support by BaCaTec.

MA 40.6 Thu 11:30 POT 081

Resonant Inelastic Light Scattering on MoS_2 — •Bastian Miller, Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching (Germany)

Two-dimensional layered 'van-der Waals' materials are of increasing interest for fundamental research due to their peculiar band-structure.

We utilize inelastic light scattering - a contactless and extremely versatile tool - to study phonon excitation spectra of mono- and fewlayer MoS_2. The phonon modes are unique fingerprints of the material properties and are sensitive to defects, strain, doping and the number of MoS_2 -layers.

We observe signatures of multistep scattering processes involving phonon-phonon, electron-phonon as well as electronic excitations under resonant conditions, where the incoming or outgoing light meets the energy of a fundamental optical transition of the system.

MA 40.7 Thu 11:45 POT 081

The effect of substrate and environment on the elementary excitations of MoS_2 — •Eric Parzinger[1], Marina Hoheneder[1], Bastian Miller[1], Anna Cattani-Scholz[1], Alexander Holleitner[1], Joel W. Ager[2], and Ursula Wurstbauer[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching (Germany) — [2]Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, California 94702 (United States)

The novel two-dimensional layered 'van-der Waals' material Molybdenum disulfide (MoS_2) is investigated using inelastic and resonant light scattering - a contactless and extremely versatile tool - to study phonon and electronic excitations. In particular, we focus on the influence of different supporting materials (SiO_2, sapphire and SAMs of organic molecules) as well as various environmental conditions (ambient, vacuum and water) on the low energy excitations of MoS_2. We

find that both, different substrate and environment give rise to a significant modification of the most prominent Raman modes, whereas a monolayer is most effected by the environmental conditions. We gratefully acknowledge financial support by BaCaTec.

MA 40.8 Thu 12:00 POT 081

Spin-orbit coupling, quantum dots, and qubits in transition metal dichalcogenides — •Andor Kormanyos[1], Viktor Zolyomi[2], Neil Drummond[2], and Guido Burkard[1] — [1]Universität Konstanz — [2]Lancaster University

We derive an effective Hamiltonian describing the dynamics of electrons in the conduction band of transition metal dichalcogenides (TMDC) in the presence of perpendicular electric and magnetic fields. We discuss both the intrinsic and Bychkov-Rashba spin-orbit coupling (SOC) induced by an external electric field. We identify a new term in the Hamiltonian of the Bychkov-Rashba SOC which does not exist in III-V semiconductors. We point out important differences in the spin-split conduction band between different TMDC compounds. A significant consequence of the strong intrinsic SOC is an effective out-of-plane g-factor for the electrons which differs from the free-electron g-factor $g \simeq 2$. Using first-principles calculations, we give estimates of the various parameters appearing in the theory. Finally, we consider quantum dots (QDs) formed in TMDC materials and derive an effective Hamiltonian allowing us to calculate the magnetic field dependence of the bound states in the QDs. We find that all states are both valley and spin split, which suggests that these QDs could be used as valley-spin filters. We explore the possibility of using spin and valley states in TMDCs as quantum bits, and conclude that, due to the relatively strong intrinsic SOC in the conduction band, the most realistic option appears to be a combined spin-valley (Kramers) qubit at low B fields.

MA 40.9 Thu 12:15 POT 081

Analytical approach to excitonic properties of MoS2 — •Gunnar Berghäuser and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We present an analytical investigation of the optical absorption spectrum of monolayer molybdenum disulfide (MoS2). Based on the density matrix formalism [1], our approach gives insights into the microscopic origin of excitonic transitions, their relative oscillator strength, and binding energy [2]. We show analytical expressions for the carrier-light coupling element, which contains the optical selection rules and well describes the valley- selective polarization in MoS2 . In agreement with experimental results, we find the formation of strongly bound electron-hole pairs due to the efficient Coulomb interaction. The absorption spectrum of MoS2 on a silicon substrate features two pronounced peaks at 1.91 eV and 2.05 eV corresponding to the A and B exciton, which are characterized by binding energies of 420 meV and 440 meV, respectively. Our calculations reveal their relative oscillator strength and predict the appearance of further low-intensity excitonic transitions at higher energies. The presented approach is applicable to other transition metal dichalcogenides and can be extended to investigations of trion and biexcitonic effects.

[1] E. Malic and A. Knorr, Graphene and Carbon Nanotubes: Ultrafast Optics and Relaxation Dynamics, 1st ed. (Wiley-VCH, Berlin, 2013).

[2] Gunnar Berghäuser and Ermin Malic, arXiv:1311.1045 (2013)