Symposium 2D Materials (SYDM)

jointly organized by
the Thin Films Division (DS),
the Semiconductor Physics Division (HL),
the Magnetism Division (MA),
the Metal and Material Physics Division (MM),
the Surface Science Division (O), and
the Low Temperature Physics Division (TT)

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The isolation of graphene in 2004 sparked the research on two-dimensional materials, which keeps growing at a tremendous rate. Since 2010 this young research area has experienced a new boost, originating from the works on graphenes' "cousins", such as transition metal dichalcogenides or MXenes. The symposium highlights the most recent advances in 2D materials and their applications, focusing on several different aspects of 2D materials research, such as nanomechanics, optics, and chemistry.

Overview of Invited Talks and Sessions

(Lecture room H 0105)

Invited Talks

SYDM 1.1	Thu	15:00–15:30	H 0105	**Bending, pulling, and cutting wrinkled two-dimensional materials** — •Kirill Bolotin
SYDM 1.2	Thu	15:30–16:00	H 0105	**Ultrafast valley and spin dynamics in single-layer transition metal dichalcogenides** — •Alejandro Molina-Sanchez
SYDM 1.3	Thu	16:00–16:30	H 0105	**Interlayer excitons in layered semiconductor transition metal dichalcogenides** — •Steffen Michaelis de Vasconcellos
SYDM 1.4	Thu	16:45–17:15	H 0105	**Exploring exciton physics in liquid-exfoliated 2D materials** — •Claudia Backes
SYDM 1.5	Thu	17:15–17:45	H 0105	**A Progress Report on Electron Transport in MXenes; A New Family of 2D Materials** — •Michel Barsoum

Sessions

SYDM 1.1–1.5	Thu	15:00–17:45	H 0105	**2D Materials**

SYDM 1: 2D Materials

Time: Thursday 15:00–17:45 Location: H 0105

Invited Talk SYDM 1.1 Thu 15:00 H 0105
Bending, pulling, and cutting wrinkled two-dimensional materials — •Kirill Bolotin — Freie Universität Berlin, Berlin, Germany

In this talk, we will examine the mechanical properties of two-dimensional materials (2DMs) using newly developed techniques to pull, bend, twist, and cut them. We will see that the mechanics of 2DMs is drastically different from that of "conventional" bulk matter. It will be shown that inevitable out-of-plane crumpling modifies every mechanical property of 2DMs making their mechanical response more akin to that of biological membranes than of solid objects. For the case of a prototypical 2DM, graphene, it will be shown that out-of-plane crumpling renders the thermal expansion coefficient negative and substrate-dependent, decreases the Young's modulus, increases the bending rigidity by several orders of magnitude, and changes the sign of the Poison's ratio. We will discuss how these unusual mechanical properties can be used in developing new types of nanomechanical devices.

Invited Talk SYDM 1.2 Thu 15:30 H 0105
Ultrafast valley and spin dynamics in single-layer transition metal dichalcogenides — •Alejandro Molina-Sanchez — Institute of Materials Science (ICMUV), University of Valencia, Spain

Single-layer transition metal dichalcogenides such as MoS_2, $MoSe_2$, WS_2 and WSe_2 are highly attractive 2D materials due to their interesting optical properties. Recent experiments have shown that a circularly polarised laser field can excite electronic transitions in one of the inequivalent K and K' valleys. Such selective valley population corresponds to a pseudospin polarization and can serve as a degree of freedom in a valleytronic device provided that the timescale for its depolarization is sufficiently large. The understanding of the photo-generation and the relaxation mechanisms is thus crucial for the use of these materials in future applications. We have developed an atomistic ab-initio methodology to simulate the valley and spin dynamics in semiconducting 2D materials. We are able to calculate the photogeneration and the subsequent relaxation of the valley polarization by several scattering mechanisms. We determine the influence of the electron-phonon interaction on the carrier and spin dynamics, the consequences of the exciton binding energy on the dynamics and the differences in the valley and spin dynamics between distinct 2D materials. Finally, we compare with ultrafast spectroscopy techniques such as time-dependent Kerr rotation and circularly polarized pump-probe experiments.

Invited Talk SYDM 1.3 Thu 16:00 H 0105
Interlayer excitons in layered semiconductor transition metal dichalcogenides — •Steffen Michaelis de Vasconcellos — Physikalisches Institut, WWU Münster, Münster, Germany

Semiconducting transition metal dichalcogenides (TMDCs) such as MoS_2, WSe_2, or $MoTe_2$ have attracted considerable attention due to their unique physical properties and their usability for novel optoelectronic devices. Unusually strongly bound electron-hole pairs, called excitons, dominate the optical and electronic properties of bulk and monolayer crystals even at room temperature.

In my talk, I will present the discovery of interlayer excitons in bulk TDMC semiconductors. Interlayer excitons, where the electron resides in one layer and the hole in the other, are very promising for achieving Bose-Einstein condensation, superfluidity, and dissipationless current flow. They have been observed in coupled GaAs quantum wells at cryogenic temperatures and artificial TMDC heterostructures. Here, we provide evidence that interlayer excitons also exist in layered bulk crystals. By combining high-field magneto-reflectance experiments and ab initio GW-BSE calculations we identify interlayer excitons in $MoTe_2$.[1] They form due to strong localization and spin-valley coupling of the charge carriers in the layers. The interlayer excitons are characterized by g-factors with opposite sign and large diamagnetic shift compared with intralayer excitons.

[1] A. Arora et al., Interlayer Excitons in a Bulk van der Waals Semiconductor, Nat. Commun. **8**, 639 (2017).

15 min. break.

Invited Talk SYDM 1.4 Thu 16:45 H 0105
Exploring exciton physics in liquid-exfoliated 2D materials — •Claudia Backes — Applied Physical Chemistry, University of Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg

Transition metal dichalcogenides (TMDSs) are a diverse source of semiconducting 2D materials interesting for number of application areas. Group VI-TMDs are direct bandgap semiconductors in the monolayer form with strongly bound exciton and trions. The physics of these excitons is of both fundamental interest and importance for exploiting these properties in applications and has been studied by optical techniques typically on micromechanically cleaved nanosheets. In this talk I will review our progress on investigating the exciton physics of layered materials exfoliated in the liquid phase. Liquid phase exfoliation has become a popular technique to obtain nanosheets in the form of colloidally stable dispersions suitable for solution processing. It is an extremely versatile technique that can be applied to a whole host of layered crystals. While dispersions of nanosheets are usually polydisperse containing broad distributions of lateral sizes and thicknesses, they can nonetheless be used to study fundamental physical properties once the distributions are quantified by statistical microscopy. The advantage of the technique is the broad applicability and characterisation of an ensemble eliminating potential variations across different nanosheets. In addition, environmental effects can be conveniently studied by exchanging the liquid environment.

Invited Talk SYDM 1.5 Thu 17:15 H 0105
A Progress Report on Electron Transport in MXenes; A New Family of 2D Materials — •Michel Barsoum — Department of Materials Science and Engineering, Drexel University, Philadelphia, USA

The 2D early transition metal carbides known as MXenes - obtained by etching the A-layers from the MAX phases, themselves layered, but strongly bonded solids - were discovered in 2011 and have generated substantial interest in the scientific community because of their potential in an ever expanding host of applications. Unlike hydrophobic graphene, MXenes are hydrophilic and behave as *conductive clays* a hitherto unknown combination. Along the same lines, because their density of states at the Fermi level is substantial, and the electric conductivity, for the most part, metal-like, MXenes can be considered as pseudo-2D metals, surface terminated by a combination of O, OH, and/or F. Said otherwise, they posses a metallic core with a hydroxide shell. It is for this reason that their proper chemical description is Mn+1XnTx, where T represents a surface termination and n = 1 to 3. In this talk, I will introduce MXenes and highlight what we currently know about their transport - which is in some cases, occurs by variable range hopping and/or thermal activation over a mobility edge - and their optical properties and how these properties relate to potential applications such as supercapacitor electrodes and electromagnetic interference shielding. The vast compositional, chemical and structural landscape that MXenes represents will be highlighted.