

# Symposium Physics of van der Waals 2D Heterostructures (SYHS)

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

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Van der Waals heterostructures based on 2D layered materials provide an exciting platform to engineer and control electronic, transport, optical properties, spin, and magnetic properties. Many exciting phenomena have been reported in stacked materials coupled by weak van der Waals interactions. Perhaps most spectacular are strong correlations and superconductivity in graphene and transition-metal dichalcogenides multilayers. Also in the exciton physics, there is a trend towards investigating signatures of many-body effects. New directions of research include searches for novel topological states, investigations of spin and magnetic proximity effects, strain physics, or studying magnetic excitations. The aim of this symposium is to present an overview of some of the recent developments in this field by leading experts in this forefront area of condensed matter physics.

## Overview of Invited Talks and Sessions

(Lecture hall HSZ 01)

### Invited Talks

SYHS 1.1	Fri	9:30–10:00	HSZ 01	<b>Novel moiré excitons and ultrafast optical dynamics in van der Waals 2D heterostructures</b> — ●STEVEN G. LOUIE
SYHS 1.2	Fri	10:00–10:30	HSZ 01	<b>Interaction induced magnetism in 2D semiconductor moiré superlattices</b> — ●XIAODONG XU
SYHS 1.3	Fri	10:30–11:00	HSZ 01	<b>Ions in tight places: intercalation and transport of ions in van der Waals heterostructures</b> — ●IRINA GRIGORIEVA
SYHS 1.4	Fri	11:15–11:45	HSZ 01	<b>Spin-orbit proximity in van der Waals heterostructures</b> — ●FELIX CASANOVA
SYHS 1.5	Fri	11:45–12:15	HSZ 01	<b>Plethora of many-body ground states in magic angle twisted bilayer graphene</b> — ●DMITRI EFETOV

### Sessions

SYHS 1.1–1.5	Fri	9:30–12:15	HSZ 01	<b>Physics of van der Waals 2D Heterostructures</b>
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## SYHS 1: Physics of van der Waals 2D Heterostructures

Time: Friday 9:30–12:15

Location: HSZ 01

**Invited Talk** SYHS 1.1 Fri 9:30 HSZ 01  
**Novel moiré excitons and ultrafast optical dynamics in van der Waals 2D heterostructures** — ●STEVEN G. LOUIE — Physics Dept, University of California, Berkeley, and Lawrence Berkeley National Lab, Berkeley, CA, USA

Recent experiments have revealed signatures of novel exciton states and intriguing pump-probe optical responses in van der Waals 2D heterostructures. But their microscopic nature remains to be fully understood. We perform ab initio GW-Bethe Salpeter equation calculations and discover a rich diversity of excitonic states in these moiré systems. In rotationally aligned WSe<sub>2</sub>/WS<sub>2</sub> heterobilayer, we find some excitons of a modulated Wannier character and others of a previously unidentified intralayer charge-transfer character. In 57.7° twisted bilayer WS<sub>2</sub>, we discover layer-hybridized excitons with in-plane charge transfer character. Many of the theoretical predictions are confirmed by experiments. Ultrafast optical dynamics in 2D heterostructures is also of fundamental and practical interest. We discover a new many-body mechanism for ultrafast photoexcited dynamics in pump-probe measurement of the optical response of transition metal dichalcogenide heterobilayers. We show that coupling between the intralayer and interlayer excitons dominates the measured ultrafast dynamics, conceptually different from a previously believed picture of single-particle charge transfer between layers. These studies are made possible with the development of two new methods that allow for the ab initio calculations of the excitonic physics and optical response of systems with thousands of atoms in the unit cell and in the time domain.

**Invited Talk** SYHS 1.2 Fri 10:00 HSZ 01  
**Interaction induced magnetism in 2D semiconductor moiré superlattices** — ●XIAODONG XU — Department of Physics, Department of Materials Science and Engineering, University of Washington, Seattle, USA

Many-body interactions between carriers lie at the heart of correlated physics. The ability to tune such interactions would open the possibility to access and control complex electronic phase diagrams on demand. Recently, moiré superlattices formed by two-dimensional materials have emerged as a promising platform for quantum engineering such phenomena. In this talk, I will present a systematic study of the emergent magnetic interactions (both antiferromagnetic and ferromagnetic) in strongly correlated transition metal dichalcogenides moiré superlattices. I will show that the combination of doping, electric field, and optical excitation provide dynamic controls of the moiré many-body Hamiltonian.

**Invited Talk** SYHS 1.3 Fri 10:30 HSZ 01  
**Ions in tight places: intercalation and transport of ions in van der Waals heterostructures** — ●IRINA GRIGORIEVA — University of Manchester, UK

Understanding and control of ion transport through angstrom-scale channels and capillaries is important in diverse technological fields, from sieving and separation to Li ion batteries and energy storage. I will review our recent work on using few-layer graphene as a model system for understanding ion intercalation in layered crystals and on ion transport through designer nanochannels made by van der Waals assembly. It allowed us to answer such questions as what limits the Li ion storage capacity of bilayer graphene, whether protons can fit into the interlayer space in van der Waals crystals, and why protons can diffuse through monolayer water while no other ions can.

15 min. break

**Invited Talk** SYHS 1.4 Fri 11:15 HSZ 01  
**Spin-orbit proximity in van der Waals heterostructures** — ●FELIX CASANOVA — CIC nanoGUNE, Donostia, Basque Country

Transition metal dichalcogenides (TMD) can be used to enhance the spin-orbit coupling of graphene, leading to new spin transport channels with unprecedented spin textures [1]. We have optimized bilayer graphene/WSe<sub>2</sub> van der Waals heterostructures to achieve magnetic-field-free spin precession. Remarkably, the sign of the precessing spin polarization can be tuned electrically by backgate voltage and drift current [2], being the first realization of a spin field-effect transistor at room temperature in a diffusive system, a long-awaited goal.

The spin-orbit proximity in graphene/TMD van der Waals heterostructures also leads to spin-to-charge conversion (SCC) of spins along z due to spin Hall effect (SHE), which was first observed by our group using MoS<sub>2</sub> as the TMD [3]. The combination of long-distance spin transport and SHE in the same material gives rise to an unprecedented figure of merit (product of spin Hall angle and spin diffusion length) of 40 nm in graphene proximitized with WSe<sub>2</sub>, which is also gate tunable [4]. Finally, we demonstrate SCC of spins oriented in all three directions (x, y, and z) in graphene/NbSe<sub>2</sub> heterostructure, due to spin-orbit proximity and broken symmetry at the twisted graphene/NbSe<sub>2</sub> interface [5].

- [1] Gmitra and Fabian, Phys. Rev. B 93, 155104 (2016)
- [2] Ingla-Aynés et al., Phys. Rev. Lett. 127, 047202 (2021)
- [3] Safeer et al., Nano Lett. 19, 1074 (2019)
- [4] Herling et al., APL Mater. 8, 071103 (2020)
- [5] Ingla-Aynés et al., 2D Mater. 9, 045001 (2022)

**Invited Talk** SYHS 1.5 Fri 11:45 HSZ 01  
**Plethora of many-body ground states in magic angle twisted bilayer graphene** — ●DMITRI EFETOV — LMU Munich, Germany

Twist-angle engineering of 2D materials has led to the recent discoveries of novel many-body ground states in moiré systems such as correlated insulators, unconventional superconductivity, strange metals, orbital magnetism and topologically nontrivial phases. These systems are clean and tuneable, where all phases can coexist in a single device, which opens up enormous possibilities to address key questions about the nature of correlation induced superconductivity and topology, and allows to create entirely novel quantum phases with enhanced interactions. In this talk we will introduce some of the main concepts underlying these systems, concentrating on magic angle twisted bilayer graphene (MATBG) and show how symmetry-broken states emerge at all integer electron fillings [1]. We further will discuss recent experiments including screened interactions [2], Chern insulators [3], magnetic Josephson junctions [4], quantum criticality [5], re-entrant correlated insulators at high magnetic fields [6], Dirac spectroscopy of correlated states in magic angle trilayers and discuss some of the avenues for novel quantum sensing applications [8].

- [1] Nature, 574, 653 (2019)
- [2] Nature, 583, 375 (2020)
- [3] Nature Physics, 17, 710 (2021)
- [4] arXiv:2110.01067 (2021)
- [5] Nature Physics, 18, 633 (2022)
- [6] PRL 128, 217701 (2022)
- [7] Nature Materials, in press (2022)
- [8] Nano Letters, 22, 6465 (2022)