

## HL 36: 2D Materials VI – Optoelectronic properties

Time: Wednesday 17:30–18:30

Location: POT/0081

HL 36.1 Wed 17:30 POT/0081

**Surface acoustic wave-controlled photocurrent in few-layer WSe<sub>2</sub>** — •BENJAMIN MAYER, FELIX EHRING, MATTHIAS WEISS, HUBERT KRENNER, URSULA WURSTBAUER, and EMELINE NYSTEN — Institute of Physics, University of Münster, Germany

Surface acoustic waves (SAWs) offer a versatile platform for nanoscience applications [1]. Their ability to integrate GHz-frequency control and sensing schemes at micron-scale wavelengths on a chip opens cross-disciplinary applications and enables the SAW electric field to drive acousto-electric currents in low-dimensional materials, including semiconducting transition metal dichalcogenides (TMDCs) [2]. Here, we study the AEC and the underlying charge-carrier dynamics in mechanically exfoliated 2D tungsten diselenide (WSe<sub>2</sub>) placed on two gold electrodes integrated into hybrid lithium-niobate-based SAW devices (150–250 MHz). Our multifunctional acousto-optoelectric setup combines current-voltage characterization, SAW-direction dependent AEC measurements and spectrally resolved scanning photocurrent (PC) spectroscopy. This allows detailed investigation of how electrical contacts affect the performance of our archetypical acoustophotovoltaic device. Thus, we establish a qualitative model of the tunneling barrier and band bending induced by Schottky barriers at the Au-TMDC interface [3]. Further, tuning the optical excitation wavelength provides spectral access to energy-dependent photocurrent contributions and reveals how they are modulated by the SAW.

[1] Krenner, J. Phys. D: Appl. Phys. (2025, subm.) [2] Nat. Comm. 6 (1): 8593 (2015) [3] ACS Appl. Electr. Mat. 7 (21): 9717 (2025)

HL 36.2 Wed 17:45 POT/0081

**Shift current tuned via twisting angle in moiré system** — •MICHELE BAGAGLINI<sup>1,2</sup>, CESARE TRESCA<sup>2</sup>, and GIANNI PROFETA<sup>1,2</sup> — <sup>1</sup>Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell’Aquila, L’Aquila, Italy — <sup>2</sup>CNR-SPIN c/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell’Aquila, L’Aquila, Italy

In recent years the interest in the two-dimensional bulk photovoltaic effect (BPVE) has been increasing in non-centrosymmetric materials. Research on 2D solar cells and optoelectronic device is focusing on these materials due to their highly efficient response. The shift current (SC) is one of the most important effect to the BPVE. The SC is second-order non-linear response that arises from the different real-space centres position of charge, a 'shift', between the valence and conduction bands. In the literature, several studies already exist on the SC in monolayer and untwisted bilayer transition-metal dichalcogenide (TMD) systems, where promising peaks have been reported from DFT calculations. In this study we focus on the evolution of the SC with the twisting angle in moiré twisted two-dimensional materials, specifically in multilayer MoS<sub>2</sub> systems. In our case, given the large size of the systems for small twist angles, we employ a tight-binding (TB) approach with Slater-Koster (SK) parameterization to compute the SC. We show that a multiband approach improves the accuracy and allows one to reproduce the dispersions obtained from first-principles calculations.

HL 36.3 Wed 18:00 POT/0081

**Theoretical investigation of the flexo-photovoltaic effect** — •JUAN JOSE ESTEVE-PAREDES<sup>1</sup>, MARIA N. GASTIASORO<sup>2</sup>, and JULEN IBANEZ-ASPIROZ<sup>1</sup> — <sup>1</sup>Materials Physics Center, University of the Basque Country, Donostia-San Sebastian, Spain — <sup>2</sup>Donostia International Physics Center, Donostia-San Sebastian, Spain

The bulk photovoltaic effect (BPVE) refers to the generation of a direct current in a bulk crystal under illumination. This phenomenon arises in non-centrosymmetric materials and is described by a finite electronic second-order conductivity. In recent years, experimental works have reported the realization of the BPVE in centrosymmetric media, where this effect is conventionally forbidden, by generating large strain gradients through application of local pressure with nanoscale tips [1,2]. This new effect, named the flexo-photovoltaic effect, has attracted interest regarding its microscopic origin. In this talk, we theoretically investigate this effect and demonstrate that a flexo-photovoltaic effect can indeed be predicted by considering local lattice deformations in several-layer centrosymmetric crystals, giving rise to the appearance of a finite BPVE conductivity. We employ a Slater-Koster approach to model the electronic band structure and wavefunctions within a supercell geometry and compute the associated linear and second-order optical responses. We discuss the tunability and scaling of this effect in relation to the magnitude and spatial extent of the mechanical deformation, and discuss how our theoretical predictions compare with existing experimental observations. [1] Yang et al., Science 360, 904 (2018) [2] Wang et al., Phys. Rev. Lett. 132, 086902 (2024)

HL 36.4 Wed 18:15 POT/0081

**All-in-one Optoelectronic Synaptic Device with Van der Waals materials-based floating gate** — •THI PHUONG ANH BACH and SANGEUN CHO — Division of System Semiconductor, Dongguk University, Seoul, South Korea

Optoelectronic synaptic devices that integrate nonvolatile memory with light matter interactions offer high processing efficiency and low energy consumption for neuromorphic computing. Two-dimensional materials and their van der Waals heterostructures provide strong electronic and optical properties, while floating-gate structures emulate synaptic plasticity and enable a path toward brain-inspired, beyond-von-Neumann computation. Herein, we demonstrate a multifunctional optoelectronic synapse device based on rhodium disulfide (ReS<sub>2</sub>)/hexagonal boron nitride (hBN)/indium selenide (InSe) vdW FG structure. The device exhibits a high On/Off current ratio ( $>10^6$ ), large memory window, multi-level storage behavior and excellent data retention ( $\sim 10000$  s) under various electrical and optical stimuli. By leveraging the thickness tunable bandgap of InSe FG and the dynamic tunneling process of photogenerated carriers across the vdW<sub>hs</sub> interface, the device capable to work under a wide range from visible to near-infrared laser with excellent synaptic plasticity. The device replicates classical conditioning (Pavlov’s dog experiment) and advanced signal-discrimination learning, and also supports reconfigurable inverter logic via electrical and optical inputs, along with neuromorphic image recognition, demonstrate its multifunctionality.