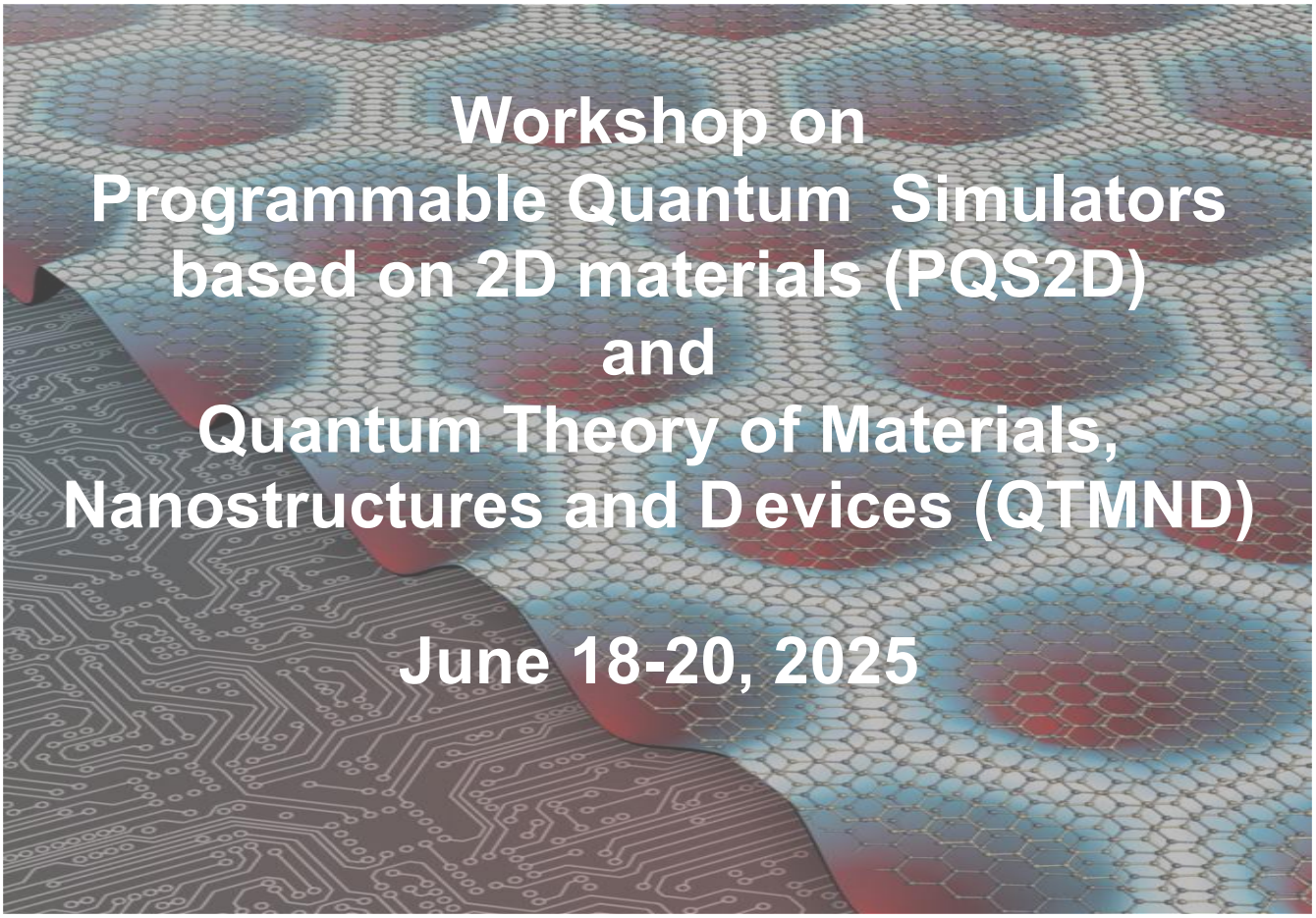
PQS2D



Workshop on Programmable Quantum Simulators based on 2D materials (PQS2D) and Quantum Theory of Materials, Nanostructures and Devices (QTMND)

June 18-20, 2025

uOttawa

UNIVERSITY OF WATERLOO

UBC

UDS Université de Sherbrooke

McGill

UNIVERSITY OF TORONTO

We welcome you to the **PQS2D/QTMND workshop** held at the Fairmont Le Château Montebello. This unique venue in Quebec is nestled along the Ottawa River, between Ottawa and Montreal.

The event merges the **Programmable Quantum Simulators based on 2D Materials (PQS2D) Annual Retreat** with the **University Research Chair in Quantum Theory of Materials, Nanostructures, and Devices (QTMND) program** from the University of Ottawa, held by Prof. Pawel Hawrylak.

These exciting three days begin on June 18 at 13:00 and conclude on June 20 at 12:10. They feature Institution Research Group Talks, Special Guest Lectures, Poster & Networking Sessions, as well as Social Events.

LOCAL ORGANIZING COMMITTEE

Justin Boddison-Chouinard, National Research Council Canada / University of Ottawa, Canada
Daniel Miravet, University of Ottawa, Canada
Didier Guignard, University of Ottawa, Canada
Marek Korkusiński, National Research Council Canada
Adina Luican-Mayer, University of Ottawa, Canada
Louis Gaudreau, National Research Council Canada / University of Ottawa, Canada
Paweł Hawrylak, University of Ottawa, Canada

SUPPORT AND FUNDING

We acknowledge uOttawa Research Chair in Quantum Theory of Materials, Nanostructures and Devices (Prof. Pawel Hawrylak)
We also acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC) – funding reference number ALLRP/578466-2022

WORKSHOP PROGRAM

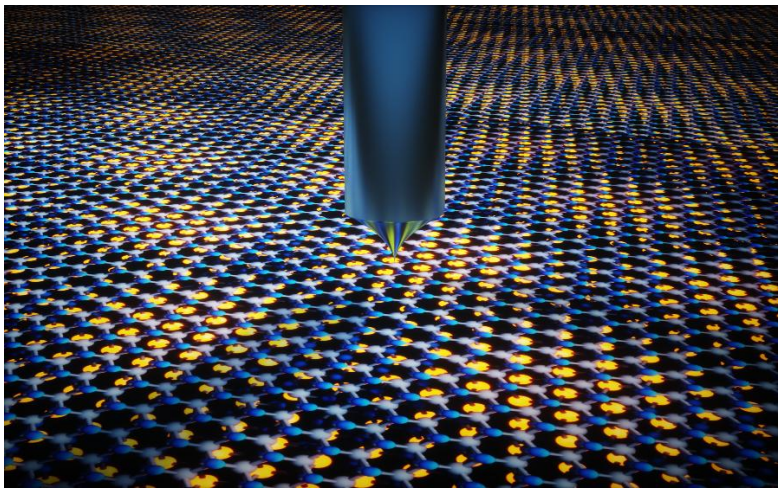
Time	Wednesday, June 18	Thursday, June 19	Friday, June 20
8:00-9:00		Breakfast	Breakfast
9:00-9:30		T1 F. Peeters	F1 C. Dean
9:30-9:50		T1 D. Guclu	F1 L. Szulakowska
9:50-10:10		T1 D. Pfannkuche	F1. S.-J. Cheng
10:10-10:30		T1 Y.-P. Shim	F1. R. Abolfath
10:30-11:00		Coffee	Coffee
11:00-11:30		T2 C. Stampfer	F2 M. Korkusinski
11:30-11:50		T2 D. Miravet	F2 O. Voznyy
11:50-12:10		T2 P. Potasz	Closing remarks
12:10-13:00		Lunch	
13:00-13:30	Welcome remarks	Lunch	
13:30-14:00	W1 A. Luican Mayer group	T3 A. Tsen group	
14:00-14:30	W1 S. de la Barrera group	T3 Z. Ye group	
14:30-15:00	W1 L. Gaudreau group	T3 P. Grutter group	
15:00-15:30	Coffee	Coffee	
15:30-16:00	W2 J. Finley	T4 M. Massicotte group	
16:00-16:30	W2 A. Wania Rodrigues	T4 J. Gerber	
16:30-16:50	W2 W. Sheng	T4 A. Delgado	
16:50-19:00	Posters/networking	Posters/networking	
19:00-21:00	Dinner	Dinner	

TALK ABSTRACTS

Visualizing Moire Structures in Twisted Semiconducting TMDs and Multilayer Graphene

Adina Luican-Mayer
Department of Physics , University of Ottawa, Ottawa
Luican-Mayer@uottawa.ca

By spanning the full range of twist angles between two-dimensional (2D) layers, one can observe the formation of long-range moire lattices or in-plane reconstructions into energetically favorable patterns. In this talk, I will discuss both phenomena in twisted transition metal dichalcogenides (TMDs) and graphene, as investigated through scanning tunneling microscopy (STM). In the first part of the talk, I will discuss the demonstration of reversible local response of domain wall networks in ferroelectric interfaces of marginally twisted WS_2 bilayers. Moreover, in the case of twisted WS_2 bilayers close to 60°, we observe signatures of at bands and study the influence of atomic relaxation on their band structure. In the second part of the talk, I will discuss recent results exploring complex moire patterns in twisted multilayer graphene.



In-situ manipulation of moiré interfaces

Sergio de la Barrera
University of Toronto, Department of Physics, Toronto, Ontario M5S 1A7, Canada
S.Barrera@utoronto.ca

The precise alignment between van der Waals layers is the critical parameter that controls the properties of moiré materials. In twisted structures, twist angle determines the length scale of the moiré periodicity, drives domain formation, and sensitively tunes emergent effects like superconductivity. Despite the importance of interlayer alignment, it is typically fixed in most samples. I will describe a method that aims to resolve this by allowing twist angle to be manipulated dynamically in a system with various electrical measurement modes.

Fully Spin Polarized Hole Transport at Low Filling Factors in Monolayer WSe2

Antoine Labbé[1,2], Justin Boddison-Chouinard[1,2], Alex Bogan[1], Pedro Barrios[1], Philip Waldron[1], Kenji Watanabe[3], Takashi Taniguchi[3], Adina Luican-Mayer[2], Louis Gaudreau[1]
[1] *National Research Council of Canada (Canada),*
[2] *University of Ottawa (Canada),*
[3] *National Institute of Material Science (Japan)*
alabb017@uottawa.ca, Louis-Gaudreau@nrc-cnrc.gc.ca, luican-mayer@uottawa.ca

One of the most promising and exciting family of two-dimensional (2D) materials is the semiconducting transition metal dichalcogenides (TMDs) [1]. Due to their 2D nature, charge carriers present in TMDs act as a 2D hole gas (2DHG) where applying a magnetic field leads to the Quantum Hall Effect [2]. Additionally, their lack of inversion symmetry at the monolayer limit and the presence of transition metals leads to opposite spins being locked to opposite valleys, also known as spin-valley locking, a phenomenon that can be leveraged for many quantum technologies [3]. Here, we introduce a device fabrication technique and architecture that enables the realization of low resistance ohmic contacts while maintaining a low carrier density in monolayer WSe_2 [4-5]. We then present magnetotransport measurements of this device and discuss the appearance of an unusual Landau fan diagram in which we observe fully spin polarized hole transport at low filling factors all the way to $\nu = 1$. We conclude by showing next generation devices that will allow greater tunability in the quantum Hall regime.

References:
[1] K. F. Mak et al., Phy. Rev. Lett. **105**, 136805 (2010).
[2] R. Pisoni, *Quantum transport in few-layer MoS_2* (PhD thesis, 2019).
[3] X. Liu and M. C. Hersam, Nat. Rev. Matter. **669** (2019).
[4] J. Boddison-Chouinard, et al., npj 2D Mater. Appl. **7**, 50 (2023).
[5] J. Boddison-Chouinard, et al., Appl. Phys. Lett. **119**, 133104 (2021).

Optically probing interacting and correlated states in electrically tunable 2D-heterostructures

A. Ben Mhenni[1], N. P. Wilson[1], A. Dijkstra[1], K. Watanabe[2], T. Taniguchi[2], S. Tongay[3], M. Knap[1], D. Van Tuan[4], H. Dery[4] and J. J. Finley[1]

[1]*Walter Schottky Institute & School of Natural Sciences, Technical University of Munich, Germany,* [2]*NIMS Tsukuba, Japan,* [3]*Arizona State University Arizona, USA,* [4]*University of Rochester, USA*

JJ.Finley@tum.de

Heterostructures formed by stacking transition metal dichalcogenide (TMD) monolayers exhibit uniquely strong Coulomb interactions and valley-contrasting physics. Such structures can sustain interacting many-body quantum states and multi-exciton complexes that can be probed using optical or electrical transport methods [1]. We will begin by exploring equilibrium Bose-Fermi mixtures in a bilayer electron system implemented in a WS_2-WSe_2 moiré heterobilayer with strong Coulomb coupling to a nearby moiré free WSe_2 monolayer [2]. As shown in Figure 1, by electrically injecting excess charges into the moiré lattice and / or proximal WSe_2 monolayer we observe signatures of correlated insulating phases in the optical response of the system. Remarkably, correlated insulating phases are found to abruptly collapse upon hole doping the moiré system with signatures of excitonic dipolar insulating phases (see Figure 1a).

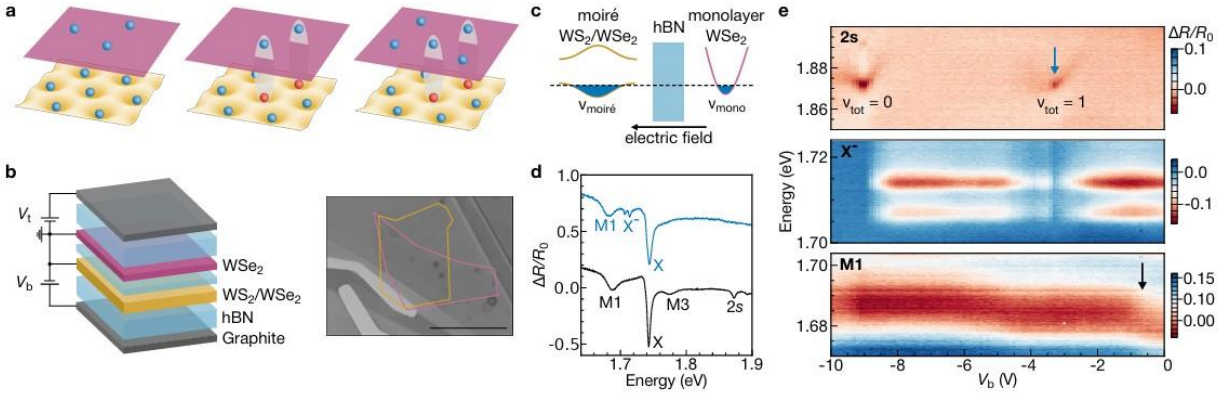


Fig. 1. Device configuration of bilayer electron system. (a) Sketch of different correlated insulating, conducting hole doped and dipolar excitonic insulator phases. (b) Schematic and optical microscope image of device – scale bar 20μm (c) Schematic band alignment, (d) Typical reflectivity spectra as a function of charge density, (e) Gate dependent reflection contrast spectrum with electron-doped WSe_2 monolayer.

In related work we probe six particle (hexciton) and eight particle (oxciton) excitonic complexes in charge tunable WSe_2 monolayers [3]. These states form due to the interaction of photoexcited electronhole pairs with electrons in multiple electrostatically induced Fermi seas, distinguishable by either spin or momentum. When following the A-hexciton with increasing electron-doping, we observe the filling of the Q - valley, resulting in a new many-body complex beyond the oxciton. Our work expands the general understanding of excitonic photo-physics in van der Waals materials.

References

[1] E. C. Regan et al. Nature Reviews Materials 7, 778 (2022).

[2] A. Ben Mhenni et al. arXiv 2410.07308, (2024).

[3] D. Van Tuan et al., Phys. Rev. Lett. 129, 076801, (2022).

Twisted graphene multilayers

A. Wania Rodrigues[1], M. Bieniek[2], D. Miravet[1], P. Potasz[3], M. Korkusinski[4], and P. Hawrylak[1]
[1]*Department of Physics, University of Ottawa, Canada*
[2]*Department of Theoretical Physics, Wrocław University of Science and Technology, Poland*
[3]*Department of Physics, Nicolaus Copernicus University in Torun, Poland*
[4]*National Research Council of Canada, Ottawa, Canada*
awaniaro@uottawa.ca

Multi-layer moiré materials offer a tunable platform for realizing electronic systems with strong electron correlations and topologically nontrivial states. We focus here on magic angle twisted bilayer and trilayer graphene, each exhibiting a flat band around the Fermi energy. In this work we determine the electronic properties of both platforms using an *ab initio* based, multi-million atomistic pz tight-binding model [1] and self-consistent Hartree-Fock (HF) method [2].

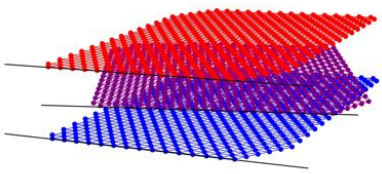


Fig.1. Mirror-symmetric twisted trilayer graphene

The electronic properties of bilayer graphene in nanoribbon geometry were determined, with the quantum size effects for the sample widths up to 1μm analyzed. For sufficiently wide ribbons, where the role of the finite geometry is minimized, we obtain and plot the Hofstadter spectrum and identify the in-gap Chern numbers by counting the total number of chiral edge states crossing these gaps. Subsequently, we examine the Wannier diagrams to identify the insulating states at charge neutrality. We establish the presence of three types of electronic states: moiré, mixed, and conventional.

In the case of trilayer, the electron-electron interactions are accounted for on the mean field level, using self-consistent Hartree-Fock (HF) method. The HF orbitals are obtained by expanding them in Bloch function for each sublattice containing a carbon atom in a unit cell and diagonalizing the large Hamiltonian matrix for each allowed wavevector self-consistently. This enabled us to determine the magnetic and topological properties of these systems as a function of the interaction strength, applied vertical electric field and presence of an hBN substrate. The tunability of these parameters provides a promising pathway to designing devices with controllable correlated and topological phases. Future work will focus on electronic correlations beyond mean field.

References

[1] A. Wania Rodrigues, M. Bieniek, P. Potasz, D. Miravet, R. Thomale, M. Korkusinski, and P. Hawrylak. Phys. Rev. B **109**, 075166 (2024).
[2] A. Wania Rodrigues, M. Bieniek, D. Miravet, and P. Hawrylak. arXiv 2501.18491 (2025).

Many-body theory of trions and its application in two-dimensional nanostructures

Weidong Sheng
Department of Physics, Fudan University, Shanghai 200433, China
shengw@fudan.edu.cn

A many-body theory of trions is presented for strongly correlated systems with an analytical expression of trion binding energy being obtained. When there are extra electrons at present, an optical excitation with lower energy may occur besides the exciton peak (X), which is usually attributed to the creation of a negatively charged exciton (X^-), commonly known as a trion. The energy difference between the X and X^- peaks was commonly regarded for the trion binding energy Δ_{X^-}, which is later however proposed to be $\Delta_{X^-} + \Delta E$ with an energy part ΔE not accurately known for decades. In this work it is deduced that $\Delta E = U_{ee} - \Delta_{qp}(N+1)$ for a confined N-electron system where U_{ee} is the interaction energy of two electrons and $\Delta_{qp}(N+1)$ is the quasiparticle gap of the system with an extra charge. By using a configuration interaction approach, the newly developed theory is applied to study the correlated trion states in phosphorene nanostructures. The energy part ΔE is shown to be crucial to obtain the trion binding energies that have the correct dielectric dependence. In the case of SiO2 substrate, our result finds that the binding energy of a negative trion in a rectangular phosphorene nanoflake with 98 atoms is around 63 meV, which agrees well with the recent experimental value of 70 meV.

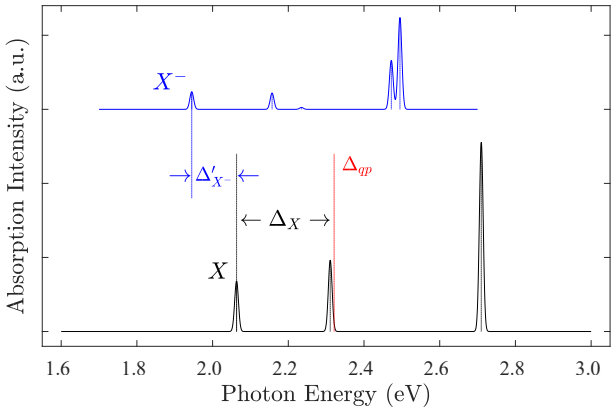


Fig. 1. Exciton and negative trion absorption peaks of a phosphorene nanoflake, together with the definitions of their binding energies.

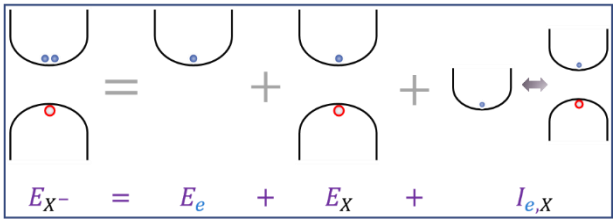


Fig. 3. Decomposition of a negative trion into an exciton with an electron in the conduction band. The difference ΔE between the norminal and real trion binding energies, Δ_{X^-} and Δ_{X^-}, are derived as $\Delta E = U_{ee} - \Delta_{qp}(N+1)$.

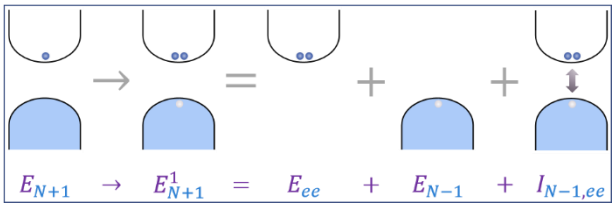


Fig. 2. Schematic depiction of trion formation: A (N+1)electron system after an excitonic excitation, consists of two parts, two electrons in the conduction band and (N−1) electrons left in the valence band. The system energy can then be decomposed into the energies of two conduction electrons and (N−1) valence electrons, and the interaction between the two parts.

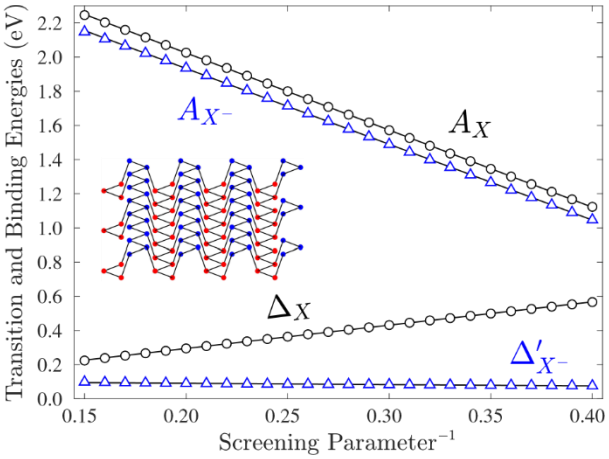


Fig. 4. Energies of the exciton (A_X) and negative trion (A_{X^-}) absorption peaks together with their energy splitting Δ'_{X^-} calculated as a function of the screening parameter for the phosphorene nanoflake as shown in the inset. For comparison, the exciton binding energy Δ_X is shown side by side with Δ_{X^-}. Linear fits are shown in solid lines.

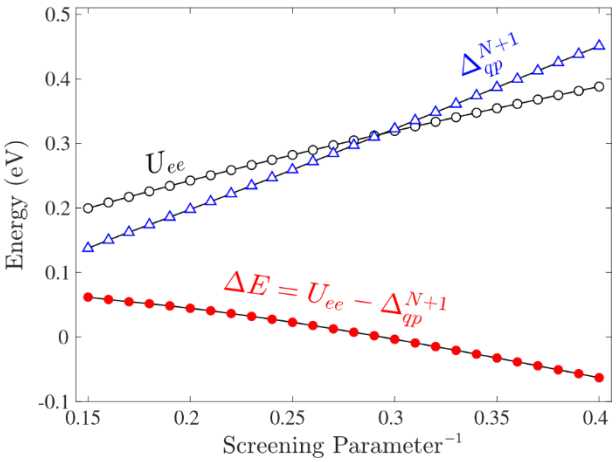


Fig. 5. Between the energy splitting Δ_{X^-} and the real binding energy of trion Δ_{X^-} lies an energy part ΔE. Two constituents of ΔE, the interaction energy between two electrons, U_{ee} and the quasiparticle gap of the system with an extra charge, $\Delta_{qp}(N+1)$ together with the energy itself, calculated as a function of the screening parameter.

Correlated quantum phases of spatially indirect excitons in heterostructures*

François Peeters
Departamento de Fisica, UFC, BR-60455900 Fortaleza, CE, Brazil
University of Antwerp, Department Physics, B-2020 Antwerpen, Belgium
Francois.Peeters@uantwerpen.be

Strongly correlated quantum phases are at the focal point of many-body physics. An important subgroup are those where fermionic pairing leads to effective Bose particles that are allowed to condense into a quantum fluid. The study of Bose condensation dates back more than half a century ago. I will present a short overview of the current status and discuss new directions. Spatially indirect excitons are promising candidates for realizing superfluidity and Bose-Einstein condensation in solid state devices. Another exotic phase is a quantum supersolid where a rigid lattice of particles flows without resistance. Within a mean-field approach we have determined the phase diagram [1] for the occurrence of Wigner crystal, exciton superfluid and exciton supersolid in the case of spatially indirect excitons in a double layer semiconductor heterostructure. Extension to anisotropic semiconductors are also considered [2].

*Work in collaboration with: S. Conti, D. Neilson, M. Milosevic, A. Perali, A. Hamilton

References

[1] S. Conti et al., Phys. Rev. Lett. **130**, 057001 (2023).
[2] J. F. de Oliveira Neto, F. M. A. Guimaraes, Davi S. Dantas, F. M. Peeters, M. V. Milosevic, and A. Chaves, *Striped excitonic (super)solid in anisotropic semiconductors with screened exciton interactions,* Phys. Rev. B (2026).

Electronic and Magnetic Properties of Semiconductor Artificial Graphene

G. Öztarhan[1], E. B. Kul[1], P. Potasz[2], E. Okcu[1] and A. D. Güçlü[1]
[1]*Department of Physics, Izmir Institute of Technology, 35430 Izmir, Türkiye*
[2]*Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Poland*
Devrim.Guclu@gmail.com

Among solid-state quantum simulators, artificial graphene, recently realized in quantum dot arrays using modulation-doped AlGaAs/GaAs quantum wells [1], has emerged as a powerful platform for exploring tunable Dirac physics and interaction-driven phenomena. The Hubbard parameter in semiconductor AG systems is predicted to be of the order of U/t ~ 100 [2], enabling the investigation of correlated insulating phases and emergent magnetism such as Nagaoka ferromagnetism [3].

In this work, we use non-perturbative quantum Monte Carlo methods complemented by exact diagonalization calculations to investigate electronic and magnetic phases of various geometries of semiconductor artificial graphene. For hexagonal geometries with armchair edges we demonstrate the emergence of Nagaoka ferromagnetism. The magnetic phase transition is driven by the absence/addition of a single electron at half-filling and stabilized by Coulomb scattering terms. For triangular geometry with zigzag edges, while the ground state at half-filling has edge polarization, we show that the depolarization of magnetic edge states by addition of a single electron overcomes Nagaoka ferromagnetism. Finally, we investigate the possibility to possibility of engineering quartic energy dispersion in honeycomb lattice structures by tuning second nearest neighbor hopping to nearest neighbor hopping via geometrical parameters. We show that it is possible to induce Mexican hat-shaped dispersion near the Γ-point.

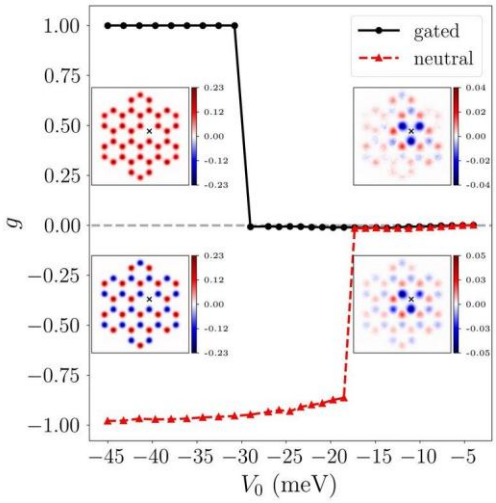


Fig. 1. Spin-spin correlation function demonstrating Nagaoka ferromagnetism.

This work was supported by The Scientific and Technological Research Council of Turkey (TUBITAK) under the 1001 Grant Project No. 119F119. The numerical calculations reported in this study were partially performed at TUBITAK ULAKBIM, High Performance and Grid Computing Center.

References

[1] S. Wang, et al. Nature Nanotech **13**, 29–33 (2018).
[2] G. Öztarhan, E. B. Kul, and A. D. Güçlü, Phys. Rev. B **108**, L161114 (2023).
[3] G. Öztarhan, P. Potasz, and A. D. Güçlü, arXiv preprint arXiv:2504.01492 (2025).

Graphene in Strong Light Fields

F. Bartelmann, M. Prada, and D. Pfannkuche
University of Hamburg, Hamburg, Germany
Frederik.Bartelmann@uni-hamburg.de

In physics, it is often the simplest models that lead to the most discoveries. In atomic physics, it is the hydrogen atom, and in condensed matter physics it is graphene. Graphene gave rise to the Haldane model and the consecutive Kane-Mele model, thereby defining the field of topological insulators. The latter, in turn, sparked countless discoveries and inventions like the ten-fold way and topological quantum computers. Now, we explore what happens if the simple condensed matter model becomes less simple. We show that by going beyond the pbands and considering the other orbitals of the carbon atoms, new phenomena can be observed. We use Floquet formalism to describe the effects of circularly polarised light on the low-lying energy bands. While doing so, we extend the work of Oka and Aoki [1] who predicted a topological phase transition of graphene into a quantum anomalous Hall insulator, as it was confirmed by McIver et al. [2].

References

[1] T. Oka and H. Aoki, Phys. Rev. B **79**. 081406 (2009).
[2] J. W. McIver, B. Schulte, F.-U. Stein, T. Matsuyama, G. Jotzu, G. Meier, and A. Cavalleri. Nature Physics, **16,** 38 (2019).

Simultaneous Control of Exchange Couplings in Quantum Dot Spin Qubit Systems

Yun-Pil Shim
The University of Texas at El Paso, El Paso, TX, USA
yshim@utep.edu

Pairwise exchange couplings have traditionally served as the primary mechanism for entangling spin qubits in semiconductor systems. However, constructing quantum circuits using only pairwise exchange gates often requires long sequences of elementary operations. In this talk, we introduce a novel approach for implementing quantum operations by simultaneously controlling multiple exchange interactions. We demonstrate this method through two representative examples: (i) the realization of three-qubit entangling gates in spin qubit systems, and (ii) a twostep protocol for implementing single-qubit gates in exchange-only qubits. Our analysis considers both linear and triangular spin configurations.

For the three-qubit gates, we derive analytical expression of an entangling gate with simultaneous exchange interactions and demonstrate its effectiveness in common quantum computing tasks, such as generating entangled states and implementing three-qubit gate like the Toffoli gate. This three-qubit entangling gate reduces the quantum circuit depth required for these tasks compared to standard approaches that rely on sequential control of pairwise exchange interactions.

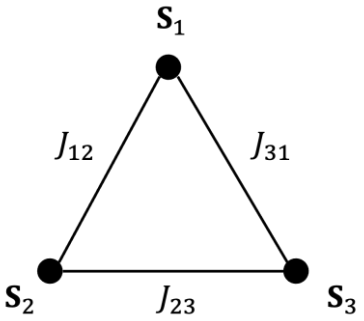


Fig. 1. Three spins coupled by exchange interactions. Simultaneous control of the exchange couplings leads to new ways of implementing entangling gates.

For an exchange-only qubit encoded in a three-spin system, the exchange interactions determine the direction of the effective magnetic field within the qubit subspace. This enables flexible control over the rotation axis for single-qubit gate operations within the xz-plane. We demonstrate that any single-qubit gate can be realized using just two rotations about axes in this plane, reducing the number of steps by up to one-third compared to the conventional Euler angle decomposition. This approach is also applicable to standard superconducting qubits (e.g., transmons), where the rotation axis for single qubit gates can be conveniently controlled via the phase of the microwave drive.

Particle–hole symmetry protected spin-valley blockade in bilayer graphene quantum dots

Christoph Stampfer
JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, Aachen, Germany
Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany
stampfer@physik.rwth-aachen.de

Particle–hole symmetry plays an important role in the characterization of topological phases in solidstate systems. It is found, for example, in free-fermion systems at half filling and it is closely related to the notion of antiparticles in relativistic field theories. In the low-energy limit, graphene is a prime example of a gapless particle–hole symmetric system described by an effective Dirac equation in which topological phases can be understood by studying ways to open a gap by preserving (or breaking) symmetries. An important example is the intrinsic Kane–Mele spin-orbit gap of graphene, which leads to a lifting of the spin-valley degeneracy and renders graphene a topological insulator in a quantum spin Hall phase while preserving particle–hole symmetry.

Here we show that bilayer graphene allows the realization of electron–hole double quantum dots that exhibit near-perfect particle–hole symmetry, in which transport occurs via the creation and annihilation of single electron–hole pairs with opposite quantum numbers. Moreover, we show that particle–hole symmetric spin and valley textures lead to a protected single-particle spin-valley blockade. The latter will allow robust spin-to-charge and valley-to-charge conversion, which are essential for the operation of spin and valley qubits.

Multielectron Complexes in Gated Bilayer Graphene Quantum Dot Arrays

D. Miravet[1], H. Allami[1], M. Korkusinski[1,2], and P. Hawrylak[1]
[1]*Department of Physics, University of Ottawa, Ottawa, Ontario, K1N 6N5, Canada*
[2]*National Research Council of Canada, Ottawa, Canada*
dmiravet@uottawa.ca

Bilayer graphene (BLG) quantum dots (QDs) have emerged as promising platforms for quantum technologies, offering electrical tunability, valley and spin degrees of freedom, and the possibility of confining electrons and holes [1,2]. This work investigates the ground-state properties of multielectron complexes confined in electrostatically defined BLG QDs, extending the study from single dots to double dots and arrays.

We begin by analyzing the case of a single BLG QD, using an atomistic tight-binding model combined with the exact diagonalization technique to solve the interacting few-electron problem. Coulomb interactions, valley mixing, and magnetic field effects are treated within the same microscopic framework, allowing us to systematically investigate spin and valley polarization transitions as functions of interaction strength and external tuning parameters. We calculate the ground state for different numbers of electrons, identifying regimes of highly correlated multielectron states.

Building on the insights from the single-dot case, we then explore coupled QDs and extend the analysis to QD arrays. Using a mapping to an effective bilinear-biquadratic (BLBQ) spin model derived from the atomistic description, we demonstrate how BLG QD arrays can emulate one-dimensional spin chains with emergent many-body phases. In particular, we identify parameter regimes where the low-energy spectrum exhibits signatures of Haldane physics, including a gapped fourfold quasidegenerate ground state and spin-1 edge excitations. The phase diagram of the effective model is mapped out, and the influence of gate-tunable parameters such as confinement potential and interdot distance is systematically explored.

Our findings provide a pathway for realizing synthetic quantum matter in electrostatically defined BLG QD arrays, with potential applications in spintronics, quantum simulators, and electrically controlled quantum information processing.

References

[1] Y. Saleem, K. Sadecka, M. Korkusinski, D. Miravet, A. Dusko, P. Hawrylak, Nano Letters **23**, 2998 (2023).
[2] M. Albert, D. Miravet, Y. Saleem, K. Sadecka, M. Korkusinski, G. Bester, P. Hawrylak, Phys. Rev. B **110**, 155421 (2024).

Analysis of optical properties of fractional Chern Insulators in moire materials

P. Potasz
Institute of Physics, Faculty of Physics, Astronomy and Informatics,
Nicolaus Copernicus University, Torun, Poland
ppotasz@umk.pl

Two-dimensional moiré superlattices have emerged as ideal systems to study the many-body interactions and correlated states. Parameters in moiré superlattices can be easily changed making them good candidates quantum simulators [1, 2]. The filling factor of the moiré energy band can be changed by varying the gate voltage, while other electronic properties can be modified by easily accessible external factors such as an external electric or magnetic fields, strain or a twist angle between the atomic layers forming a moiré pattern. Various many-body interacting states have already been engineered, such as Mott insulator states at one hole per superlattice unit cell, superconductivity, generalized Wigner crystal states, different charge orders or, very recently, fractional Chern insulators at partial fillings of topologically non-trivial energy bands. These fractionalized states in moiré systems are expected to be in the same universality class as their counterparts in Landau levels, but the periodic potential and quantum geometry can have significant effects on physical observables.

In this work, we analyze how the properties of fractional Chern insulators differ from those of standard fractional quantum Hall (FQH) states in a Landau level. We determine ideal quantum geometry conditions where Landau-level-like correlations at long length scales are expected [3, 4]. Here, it was recently shown that intraband collective excitations in fractional Chern insulators are dark [5]. Moving away from this ideal point by varying model parameters, we investigate the effect of quantum geometry on collective excitations of FCI's and their coupling to light. We show how the THz absorption characteristics of FCI and FQH states can be tuned by varying a moiré twist angle or by the displacement field. Our numerical calculations are performed using exact diagonalization method and dynamical correlation functions are obtained using Lanczos method.

References

[1] D. Kennes et al., Nature Phys. **17**, 155 (2021).
[2] F. Wu, T. Lovorn, E. Tutuc, and A. H. MacDonald, Phys. Rev. Lett. **121**, 026402 (2018).
[3] R. Roy, Phys.Rev. B **90**, 165139 (2014).
[4] S. A. Parameswaran, R. Roy, and S. L. Sondhi, Phys. Rev. B **85**, 241308 (2012).
[5] T. Wolf, Y.-C. Chao, A. H. MacDonald, and J.-J. Su, Phys. Rev. Lett. **134**, 116501 (2025).

Charge, Spin, and Symmetry in a 2D Topological Semimetal

Adam W. Tsen
University of Waterloo
awtsen@uwaterloo.ca

Low-symmetry two-dimensional (2D) topological materials such as $MoTe_2$ host efficient charge-to-spin conversion (CSC) mechanisms that can be harnessed for novel electronic and spintronic devices. Yet, the nature of the various CSC mechanisms and their correlation with underlying crystal symmetries remain unsettled. I will discuss our recent results using local spin-sensitive electrochemical potential measurements to directly probe the spatially dependent nonequilibrium spin accumulation in $MoTe_2$ across various sample locations and thicknesses. We uncover an abundance of unconventional spin polarizations that develop uniquely in the sample bulk and edges with decreasing thickness. Using *ab initio* calculations, we construct a unified understanding of all the observed CSC components in relation to the material dimensionality and stacking arrangement. Our findings both illuminate previous CSC results on $MoTe_2$ and have important consequences for the design of future devices utilizing this 2D topological material.

Correlated Insulating States Induced by Honeycomb Moiré Superlattice in Twisted $MoSe_2$ Bi-layer

Dongyang Yang[1,2,†], Jing Liang[1,2,†], Haodong Hu[1,2,†], Nitin Kaushal[1,2], Kenji Watanabe[3], Takashi Taniguchi[4], Jerry. I Dadap[1,2], Marcel Franz[1,2], and Ziliang Ye[1,2,*]

[1]*Department of Physics and Astronomy, The University of British Columbia, Vancouver, BC, V6T 1Z1, Canada*
[2]*Quantum Matter Institute, The University of British Columbia, Vancouver, BC, V6T 1Z4, Canada*
3Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan
4International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan
[†]These authors contribute equally to this work
[*]Corresponding author: zlye@phas.ubc.ca

When two layers of certain transition metal dichalcogenide are stacked with a small relative twist angle, a honeycomb superlattice is formed, giving rise to a graphene-like Moiré band structure with a much slower Fermi velocity. In such an artificial graphene, the significantly reduced kinetic energy of a single electron becomes comparable to the Coulomb repulsion energy between electrons, rendering the system an ideal platform for studying strongly correlated Dirac fermions. In this work, we experimentally study the twisted $MoSe_2$ homobilayer where Moiré flatbands are folded from the Gamma valley of the constituent layer where the spin-orbital coupling is negligible. By leveraging the Rydberg exciton sensing technique, we observe correlation-induced Mott gap opening at the Dirac point, persisting up to 110 K, together with a series of insulating states at other integer and fractional fillings. Interestingly, we find that the two insulating states at integer fillings exhibit distinct magnetic responses. One state is paramagnetic with weak ferromagnetic coupling, while the other displays vanishing magnetic susceptibility. Furthermore, we identify two distinct types of Moiré trions with unique real-space configurations, which allows us to resolve the charge distributions at these fillings. Our work highlights the potential of simulating a wide range of quantum many-body phenomena in twisted two-dimensional materials.

Measuring properties of single defects, dopants and quantum dots with nm spatial resolution

Megan Cowie[1], Taylor J.Z. Stock[2,3], Procopios C. Constantinou[2], Neil J. Curson[2,3], and Peter Grutter[1]
[1]*Department of Physics, McGill University, Montreal, Quebec, Canada*
[2]*London Centre for Nanotechnology, University College London, London, UK*
[3]*Department of Electronic and Electrical Engineering, University College London, London, UK*
Corresponding email: Peter.Grutter@mcgill.ca

Semiconductor interfaces often have isolated trap states which modify electronic properties. We have developed a framework to quantitatively describe a metal-insulator semiconductor (MIS) device formed out of a metallic AFM tip, vacuum gap, and semiconducting sample. This framework allows the measurement of local dopant concentration, bandgap and band bending timescales with nm scale resolution of different types of defects on semiconductors such as Si, 2D $MoSe_2$ and pentacene monolayers [1].

With this method, we have characterized individual defects at the Si-SiOx interface. We show that surface charge equilibration timescales, which range from 1−150 ns, increase significantly around interfacial states [2]. We conclude that dielectric loss under time-varying gate biases at MHz and sub-MHz frequencies in metal-insulator-semiconductor capacitor device architectures is highly spatially heterogeneous over nm length scales. We have also analyzed two-state fluctuations localized at these interfacial traps, exhibiting bias-dependent rates and amplitudes. When measured as an ensemble, these observed defects have a 1/f power spectral trend at low frequencies [3]. Low-frequency noise due to two level fluctuations inhibits the reliability and performance of nanoscale semiconductor devices, and challenges the scaling of emerging spin based quantum sensors and computers. The presented method and insights provide a more detailed understanding of the origins of 1/f noise in siliconbased classical and quantum devices, and could be used to develop processing techniques to reduce two-state fluctuations associated with defects.

Force detection with single electron sensitivity can be used to perform localized electron energy level spectroscopy on semiconductor quantum dots, individual ferrocene molecules and atomically precisely positioned dopant atoms in Si. Single electron force spectroscopy allows the measurement of Coulomb blockade and eigen state energy levels, shell structure, excited state energies, coupling strength to electrodes, molecular vibrations, reorganization energies, electron-nuclear coupling (Franck-Condon blockade), stability diagrams (i.e. coupling between qdots) and double dot coherence time (for a recent review see [4]). I will describe the challenges and progress towards applying this single electron force spectroscopy technique to atomically precisely positioned quantum dots in Si.

References:
[1] M. Cowie, et al., Phys. Rev. Materials **6**, 104002 (2022)
[2] M. Cowie, et al., Phys. Rev. Lett. **132**, 256202 (2024)
[3] M. Cowie, et al., Proc. Natl. Acad. Sci. USA **121** (44) e2404456121 (2024)
[4] Y. Miyahara, et al., Nanotechnology **28**, 064001 (2017)

Refined Large-Area Graphene Transfer for Semiconductor Integration

R. J. Mathew[1,2,3], L. Farmanel[1], M. Hérisson de Beauvoir[1], M. Ivanauskas[1],
F. Banville[3], S. Ecoffey[2,3] and M. Massicotte[1,2,3*]
[1]*Institut quantique, Université de Sherbrooke, QC, Canada*
[2]*Département de génie électrique et génie informatique, Université de Sherbrooke, QC, Canada*
[3]*Institut Interdisciplinaire d'Innovation Technologique (3IT), Laboratoire Nanotechnologies et Nanosystèmes (LN2) - CNRS IRL-3463, QC, Canada*
*Mathieu.Massicotte@usherbrooke.ca

Integrating two-dimensional (2D) materials like graphene into industrial applications hinges on scalable, highyield transfer methods that preserve material quality and ensure compatibility with diverse substrates. The conventional wet transfer methods, which rely on polymer supports introduce uncontrollable contamination due to residual polymer and etchant residues, creating unintentional doping, structural defects arising from cracks or wrinkles, deteriorating the electronic properties, and limited scalability for mass semiconductor production. This work introduces a refined metal-assisted graphene transfer technique, leveraging a metal thin film and thermal release tape stack for seamless graphene transfer. The metal-assisted approach offers a quasi-dry, residue-free preferential transfer/printing process with enhanced scalability control. The dry graphene-substrate interface and the controlled etching of metal achieve clean graphene transfer, mitigating the conventional wet transfer issues.

Raman spectroscopy confirms the preservation of graphene's structural integrity post-transfer. This method offers uniformity and reproducibility, minimal contamination and defect density, high carrier mobility retention, high throughput and scalability, economic viability, and integration compatibility with other semiconductor fabrication processes, as demonstrated by successful integration onto pre-patterned substrates. We discuss the method's advantages and its applicability to other 2D materials, including hBN and transition metal dichalcogenides. The proposed technique offers a pathway for broader adoption of 2D materials in next-generation device manufacturing.

Probing anisotropic magnetism in few-layer α-$RuCl_3$ via electron tunneling

M. Massicotte[1,2], S. Dehlavi[1], X. Liu[3], J. L. Hart[4], E. Garnaoui[1], P. Lampen-Kelley[5], J. Q. Yan[5], D. Mandrus[5], S. E. Nagler[6], K. Watanabe[7], T. Taniguchi[7], B. Reulet[1], J. J. Cha[4], H.-Y. Kee[3], J. A. Quilliam[1]

[1] *Institut quantique, Département de physique, Université de Sherbrooke, Sherbrooke, QC, J1K 2R1, Canada*
[2] *Institut Interdisciplinaire d'Innovation Technologique, Laboratoire Nanotechnologies Nanosystèmes – CNRS, Département de génie électrique et génie informatique, Université de Sherbrooke, Sherbrooke, J1K 2R1, Canada*
[3] *Department of Physics, University of Toronto, Toronto, Ontario, M5S 1A7, Canada*
[4] *Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853, USA*
[5] *Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA and Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996*
[6] *Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA and Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996, USA*
[7] *National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*
Mathieu.Massicotte@usherbrooke.ca

The magnetic insulator α-$RuCl_3$ is proximate to a quantum spin liquid (QSL) [1] described by the Kitaev model [2]. A promising route to realizing a true Kitaev QSL in α-$RuCl_3$ is to reduce its dimensionality via mechanical exfoliation. In addition to enhancing magnetic fluctuations, exfoliating α-$RuCl_3$ opens the door to manipulating its magnetic state by coupling it to other two-dimensional materials. Here, we present angle-dependent tunneling magnetoresistance (TMR) measurements on ultrathin α-$RuCl_3$ crystals with various layer numbers to probe their magnetic, electronic and crystal structure. We observe a giant change in resistance – as large as $\sim$ 2500 % – when the magnetic field rotates either within or out of the α-$RuCl_3$ plane. This is a manifestation of the anisotropic spin interactions arising from the strong spin-orbit coupling in this material. Using TMR as a probe, we track the magnetic phase diagram of few-layer α-$RuCl_3$, which reveals an AFM ground state with a Néel temperature twice as high as the one of most bulk crystals. Our study provides a deeper understanding of how the magnetic properties of α-$RuCl_3$ depend on its stacking order and layer number, which helps lay the groundwork for the van der Waals engineering of exotic magnetic phases such as QSLs.

References:
[1] Takagi, H. *et al*. *Nat. Rev. Phys*. **1**, 264–280 (2019).
[2] Kitaev, A. *Ann. Phys.* **321,** 2-111 (2006).
[3] Massicotte, M. *et al*. *ACS Nano*, **18**, 25118–25127 (2024).

Enhanced and Tunable Spin-Orbit Splitting in Bilayer Graphene Quantum Devices

J. Gerber*[1], E. Ersoy[1], M. Masseroni[1], M. Niese[1], M. Laumer[2], A. Denisov[1], H. Duprez[1], W. Huang[1], C. Adam[1], L. Ostertag[1], C. Tong[1], T. Taniguchi[3], K. Watanabe[4], V. Fal'ko[5], T. Ihn[1], K. Ensslin[1], A. Knothe[2]

[1]*Solid State Physics Laboratory, ETH Zürich, 8093 Zürich, Switzerland*
[2]*Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany*
[3]*Research Center for Materials Nanoarchitectonics, 1-1 Namiki, Tsukuba 305-0044, Japan*
[4]*Research Center for Electronic and Optical Materials, 1-1 Namiki, Tsukuba 305-0044, Japan*
[5]*National Graphene Institute, University of Manchester, Manchester M13 9PL, UK*
*gerberjo@phys.ethz.ch

Bilayer graphene (BLG) has emerged as a promising platform for quantum information technologies due to its electrically tunable band gap [1], high carrier mobility [2], and absence of nuclear spins [3]. Recent experiments have demonstrated spin-valley relaxation times exceeding 30 seconds in BLG-based quantum dots [4], underscoring its potential for spin qubits. For applications in quantum computing, strong spin–orbit coupling (SOC) is desirable to enable all-electrical spin control, such as electric dipole spin resonance [5]. However, the intrinsic SOC in BLG is weak, with spin-orbit splitting in the range of 40–80 μeV [6,7].

Here, we demonstrate a significant enhancement of spin-orbit splitting—by more than an order of magnitude (up to 1.5 meV)—by proximitizing BLG with a layer of WSe_2. Using both quantum dots and quantum point contacts in two different BLG/WSe_2 stacking configurations, we probe the SOC and show its in situ tunability via an external electric field, which modulates layer polarization. [8]

These findings establish proximity-induced and electrically tunable SOC in BLG/WSe_2 as a powerful mechanism for dynamic spin and valley control in scalable quantum devices.

References

[1] Oostinga *et al*. Nat. Mater. **7**, 151 (2008).
[2] Wang *et al*. Science **342**, 614 (2013).
[3] Trauzettel *et al*. Nat. Phys. **3**, 192 (2007).
[4] Denisov *et al*. Nat. Nanotechnol. 10.1038/s41565-025-01858-8 (2025).
[5] Hendrickx *et al*. Nature **577**, 487 (2020).
[6] Banszerus *et al*. Phys. Rev. Lett. **124**, 177701 (2020).
[7] Kurzmann *et al*. Nat. Commun. **12**, 5250 (2021).
[8] Gerber *et al*. ArXiv:2504.05864 (2025).

Quantum Simulations of the Spectral Properties of Materials

S. Fomichev, P. Casares, A. Kunitza, T. Stetina, I. Loaiza, D. Motlagh, A. Delgado, J.M. Arrazola
Xanadu, Toronto, Ontario, M5G 2C8, Canada
alaindelgado@xanadu.ai

Quantum computers have the potential to overcome the limitations of classical methods for simulating the spectral properties of materials involving excited states. However, considerable progress still needs to occur on both quantum hardware and quantum algorithms to make this promise a reality. In this talk I will provide an overview of the quantum algorithms developed at Xanadu for spectroscopy applications. I will show how they leverage the quantum computer to efficiently perform the time evolution of a prepared initial state to recover the spectrum of interest. The main algorithmic subroutines and the optimizations used to reduce the cost of the simulations are described. The usefulness of the algorithms is demonstrated through concrete applications, including X-ray and electron energy loss spectroscopy of battery materials [1-2], near-infrared spectroscopy of molecules [3], and the optical response of spin defects [4]. The estimated number of logical qubits and gates required to perform quantum simulations of the investigated materials are discussed. Finally, I provide an outlook on future work.

References

[1] R.A. House *et al*., Nature Energy **8**, 351 (2023); X. Gao *et al*., *Nature Materials* (2025), https://doi.org/10.1038/s41563-025-02144-7.
[2] S. Fomichev *et al*., arXiv:2405.11015.
[3] I. Loaiza *et al*., arXiv:2504.10602.
[4] J.S. Baker *et al*., Phys. Rev. A 110, 032606 (2024).

Superconductivity in twisted bilayer WSe_2

C. Dean
Department of Physics, Columbia University, New York, NY, USA
cd2478@columbia.edu

Superconductivity in twisted bilayer and twisted trilayer graphene results from an interplay between interlayer coupling and a moiré superlattice that gives rise to low-energy flat bands with strong correlations. Similar flat bands have been explored in lattice-mismatched and or twisted heterostructures of other two-dimensional materials beyond graphene such as transition metal dichalcogenides (TMDs). However, despite a wide range of correlated phenomenon robust demonstration of superconductivity in the TMDs remained absent and its possibility an open question. In my talk I will discuss our recent observation of superconductivity in twisted bilayer WSe2 at relatively large twist angles near 5 degrees. The superconducting state appears in a limited region of displacement field and density that is adjacent to a metallic state with Fermi surface reconstruction believed to arise from antiferromagnetic order. A sharp boundary is observed between the superconducting and magnetic phases at low temperature, reminiscent of spin-fluctuation mediated superconductivity. Our results establish that moiré flat-band superconductivity extends beyond graphene structures. Material properties that are absent in graphene but intrinsic among the TMDs such as a native band gap, large spin-orbit coupling, spin-valley locking, and magnetism offer the possibility to access a broader superconducting parameter space than graphene-only structures.

Exciton theory for self-organised quantum dots in marginally twisted TMDC bilayers

L. Szulakowska[1,2], I. Soltero[1], J. McHugh[1], V. Falko[1]
[1]*National Graphene Institute, University of Manchester, Manchester, UK*
[2]*Quantinuum, Terrington House, 13-15 Hills Road, Cambridge CB2 1NL, UK*
Ludmila.Szulakowska@gmail.com

Multilayer transition metal dichalcogenides (TMDCs) have emerged as an attractive platform for designing optoelectronic devices due to their strong light-matter interaction [1], long-lived excitons [1] and convenient band gap control using strain or electric bias [2]. In this work we present the exciton theory in self-organised quantum dots formed at the domain boundaries of the reconstructed lattice of marginally twisted bilayers of TMDCs.

When type-II bilayers of TMDCs are marginally twisted, the lattice strain from reconstruction competes with adhesion energy gain from favourable lattice stackings. In effect, the areas of low adhesion energy dominate the material, and they are interrupted by a differently stacked network of domain walls [3, 4]. At the nodes of this network, strain hot spots create quantum dots (QDs) that can host electrons and holes. Together with TMDCs strong optical response, this easily fabricated uniform nanoscale grid offers a promising perspective for indistinguishable photon emission for photonic applications [1,3].

To study the excitonic properties in these materials, we first obtain the single particle (SP) QD energy levels by using the strain-induced piezoelectric potential modulating the valence and conduction band profiles. We then populate the SP energy levels with electrons and holes, calculate the Coulomb matrix elements and build the Hamiltonian matrix in the basis of electron-hole excitations. To compute the electron-electron interaction terms we assume an anisotropic surrounding medium and consider a strongly screened multilayer Keldysh-based interaction model [1]. We then solve the Bethe Salpeter equation to obtain the QD exciton states and their binding energies. We report the range of twist angles for which the excitons localise within the QDs and the optical selection rules for different valley and light polarisation [1,3,5]. For all heterostructures, we mark the transition of exciton states to the quantum-wire domain boundaries and to the lattice domains.

References

[1] M. Danovich, D. A. Ruiz-Tijerina, R. J. Hunt, M. Szyniszewski, N. D. Drummond, V. I. Fal'ko, Phys. Rev. B **97**, (2018) 195452.
[2] L. A. Jauregui et al., Science, **366**, 6467, (2019) 870–875.
[3] V. V. Enaldiev, F. Ferreira, J. G. McHugh, Vladimir I. Fal'ko, npj 2D Mat. & App. **6** (2022).
[4] I. Soltero, M. A. Kaliteevski, J. G. McHugh, V. Enaldiev, V. I. Fal'ko, Nano Lett. **24**, 6, (2024) 1996–2002.
[5] J. Hagel, S. Brem, J. A. Pineiro, E. Malic, Phys. Rev. Mat. **8**, (2024) 034001.

Landscape of Finite Momentum Excitons in Atomically thin Transition-metal Dichalcogenides

Shun-Jen Cheng
Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu 300, Taiwan
sjcheng@nycu.edu.tw

In this work, we shall review our recent theoretical investigations of finite momentum excitons in atomically thin transition-metal dichalcogenides (TMDs), including single and few monolayers, by using the in-house code of Bethe-Salpeter equation (BSE) solver, *WannierBSE*.[1] Combined with open-access first-principles packages, e.g. Quantum Espresso, and Wannier90, the *WannierBSE* package can establish and efficiently solve the DFT-based BSE in the Wannier tight binding (WTB) scheme for exciton complexes, exciton and trion, in 2D materials.

By employing *WannierBSE,* we calculate and present the full-zone band structures and momentum dependent valley polarizations of exciton in a WSe2 monolayer, showing intriguing topological texture landscape of valley polarization over the extended reciprocal space. The symmetry analysis of the momentum-dependent texture of valley polarization identifies the intrinsic depolarization nature of intra-valley bright exciton, and reveals the symmetry-sustained robustness of high degree of valley polarization of inter-valley excitons, [2] as observed in experiments.

Increasing the number of monolayers, the intervalley excitons with large momentum emerges as the ground state excitons in multilayer TMDs. Remarkably, inter-valley excitons are paired by the time reversal counter parts with opposite exciton momenta, valley polarizations and spin orientations. With long lifetimes and opposite momenta, pairs of time-reversed inter-valley excitons in multi-layer TMDs are shown likely annihilated by each other and up-converted to a high energy bright exciton with zero momenta. Such an exciton-exciton annihilation of intervalley dark exciton has been for the first time evidenced by our experiment-theory-joint studies of the observed up-converted photoluminescence from multi-layer TMDs. [3]

References:

[1] Guan-Hao Peng, Ping-Yuan Lo, Wei-Hua Li, Yan-Chen Huang, Yan-Hong Chen, Chi-Hsuan Lee, Chih-Kai Yang, Shun-Jen Cheng. *Distinctive Signatures of the Spin- and Momentum-Forbidden Dark Exciton States in the Photoluminescence of Strained WSe2 Monolayers under Thermalization*. Nano Letters **19**, 2299 (2019); https://quantum.web.nycu.edu.tw/wannierbse/

[2] Ping-Yuan Lo, Guan-Hao Peng, Wei-Hua Li, Yi Yang, Shun-Jen Cheng* (2021, Nov), *Full-zone valley polarization landscape of finite-momentum exciton in transition metal dichalcogenide monolayers*, Phys. Rev. Research **3**, 043198 (2021).

[3] Yi-Hsun Chen, Ping-Yuan Lo, Kyle W Boschen, Chih-En Hsu, Yung-Ning Hsu, Luke N Holtzman, Guan-Hao Peng, Chun-Jui Huang, Madisen Holbrook, Wei-Hua Wang, Katayun Barmak, James Hone, Pawel Hawrylak, Hung-Chung Hsueh, Jeffrey A Davis, Shun-Jen Cheng, Michael S Fuhrer, Shao-Yu Chen, *Efficient light upconversion via resonant exciton-exciton annihilation of dark excitons in few-layer transition metal dichalcogenides.* Nature Communications **16** (1), 2935 (2025).

Applications for quantum materials, nano-devices and quantum simulators in FLASH ultra-high dose rate radiotherapy: opportunities and challenges

Ramin Abolfath[1,2]
[1]*Department of Physics and Astronomy, Howard University, Washington, DC 20059, USA*
[2]*Department of Radiation Physics and Oncology, University of Texas MD Anderson Cancer Center, Houston, TX, 75031, USA*
Ramin.Abolfath@howard.edu

Quantum materials, nano-devices, and quantum simulators offer exciting possibilities for advancements in radiotherapy, particularly in areas like precision beam characterization, dosimetry, targeting, enhanced imaging, and possibly improved patient treatment planning and personalized medicine. Clinical outcomes and gains of therapeutical applications of ionizing radiation to treat and control cancer with minimum toxicity to normal tissues rely on (1) mathematical model predictions and multi-scale computational approaches that bridge molecular level interactions and system-level network dynamics, and (2) beam characterization and measurement. Quantum chemistry describes accurately the underlying microscopic mechanisms of biological responses of interacting cells and organisms under exposure of ionizing radiation. Whereas quantum sensing by nano-structure devices may help to deconvolve the spatial and temporal distribution of fast-moving charges particles to understand hypothetical correlations in reaction and diffusion of the reactive oxygen species in normal and cancerous cells. Particularly in the limit of ultra-high dose rates where the standard dosimetry techniques have resulted in under-responsive signals due to quenching and excessive recombination of ions and molecular excitations. In this talk, I briefly highlight the current challenges in FLASH radiotherapy [1, 2] in which quantum technologies and algorithms can potentially lead to more effective and less toxic outcomes for treatments of cancer.

References

[1] Ramin Abolfath, Sedigheh Fardirad, Houda Kacem, Marie-Catherine Vozenin, Abbas Ghasemizad, *A Monte Carlo simulation framework for investigating the effect of inter-track coupling on H2O2 productions at ultra-high dose rates*, Medical Physics, under publication, arXiv:2403.16722v3.
[2] Ramin Abolfath, Niayesh Afshordi, Sohrab Rahvar, Adri van Duin, Martin Radler, Julie Lascaud, Reza Taleei, Katia Parodi, Radhe Mohan, *A molecular dynamics simulation framework for investigating ionizing radiation-induced nano-bubble interactions at ultra-high dose rates*, Eur. Phys. J. D **78**:141 (2024), https://doi.org/10.1140/epjd/s10053-024-00928-1.

Theory of excitons, trions, and highly charged magnetoexcitons confined in a gated bilayer graphene quantum dot and in two-dimensional TMDCs

M. Korkusinski[1,3], D. Miravet[1], K. Sadecka[1,2], Y. Saleem[1,5], M. Albert[1,4], M. Bieniek[2], and P. Hawrylak[1]
[1]*Department of Physics, University of Ottawa, Ottawa, Canada*
[2]*Institute of Theoretical Physics, Wroclaw University of Science and Technology, Wroclaw, Poland*
[3]*Quantum and Nanotechnologies, National Research Council, Ottawa, Canada*
[4]*Department of Physics, University of Toronto, Toronto, Canada*
[5]*Condensed Matter Theory, Department of Physics, TU Dortmund, Dortmund, Germany*
Marek.Korkusinski@nrc-cnrc.gc.ca

There is currently interest in quantum dots (QDs) as building blocks of quantum circuits and nanophotonic devices. Following the development of QDs based on semiconducting materials, a new class of two-dimensional (2D) semiconductors was developed based on 2D materials, including bilayer graphene (BLG) [1-4]. In the BLG, an energy gap opens by applying a vertical electric displacement field, paving the way towards lateral electrical confinement of carriers. The energy gap can be tuned electrically in the terahertz to far infrared (FIR) range [2, 4]. Moreover, unlike in laterally gated semiconductor QDs, attracting only one carrier type and repelling another, in a BLG QD it is possible to confine electrically both electrons and holes [2, 4].

Here we present a theory of electronic and optical properties of neutral and charged excitonic complexes confined in a BLG QD at zero and finite magnetic field [2, 4, 5]. We utilize the atomistic tight-binding approach to compute the single-particle energies and wave functions of quasiparticles confined in a BLG QD consisting of ~1.6 million atoms, followed by the microscopic calculation of Coulomb and dipole matrix elements. This allows us to formulate a Hamiltonian of interacting quasiparticles accounting for the BLG valleys, trigonal warping, and details of the displacement and lateral confinement potentials on equal footing.

We consider a strongly interacting exciton X, a biexciton XX, and a negatively charged trion X- confined in the BLG QD by solving the Bethe-Salpeter equation [2, 4, 5]. We find their energies to be tunable by voltage from the terahertz to FIR range. The conservation of spin, valley, and orbital angular momentum results in an X, XX, and X- fine structure with a band of dark low-energy states, making this system a promising candidate for constructing nanodevices for storage, emission and detection of photons in the terahertz range.

We extend our description to consider the emission spectra of excitons accompanied by zero, one, and many electrons in a two-dimensional transition metal dichalcogenide in strong magnetic fields [6]. Utilizing the massive Dirac Fermion model specialized to MoS_2 we first establish the structure of Landau levels and the optical selection rules governing the emission process. We then proceed to considering the electronic properties of a single electron-hole pair, a singly charged exciton, and an exciton immersed in a two-dimensional electron gas in the $\nu = 1$ state utilizing the Bethe-Salpeter approach. We then predict the emission spectra as a function of the magnetic field, temperature, and density of the additional carriers in the conduction band. As the electron density increases, we observe (i) a redshift of emission maxima as a result of exchange interactions with the electron gas, and (ii) a broadening of the maxima owing to the increasingly correlated nature of many-body states.

References

[1] D. Guclu, P. Potasz, M. Korkusinski, and P. Hawrylak, *Graphene Quantum Dots*, Springer-Verlag (2014).
[2] Y. Saleem, K. Sadecka, M. Korkusinski, D. Miravet, A. Dusko, and P. Hawrylak, Nano Lett. **23**, 2998 (2023).
[3] D. Miravet, L.Szulakowska, M. Bieniek, M. Korkusinski, P. Hawrylak, Phys. Rev. B **110**, 235404 (2024).
[4] M. Albert, Y Saleem, K Sadecka, M Korkusinski, D Miravet, P Hawrylak, Phys. Rev. B **110**, 155421 (2024).
[5] K. Sadecka, Y. Saleem, D. Miravet, M. Albert, M. Korkusinski, G. Bester, and P. Hawrylak, Phys. Rev. B **109**, 085434 (2024).
[6] L. Szulakowska, M. Bieniek, and P. Hawrylak, Solid State Electronics **155**, 105 (2019).

Semi-empirical and machine learning methods for accelerating quantum theory of nanostructures

O. Voznyy[1]
[1]*University of Toronto Scarborough, Scarborough, Ontario M1C 1A4, Canada*
O.Voznyy@utoronto.ca

Accurate quantum mechanical simulations are indispensable for understanding and designing nanostructures, from semiconductor quantum dots to 2D materials. While **Density Functional Theory** (DFT) provides a robust framework, its computational cost becomes prohibitive for systems exceeding a few hundred atoms – a scale routinely encountered in realistic models of surfaces, ligand-functionalized nanoparticles, or catalytic interfaces.

Our exploration of state-of-the-art "brute-force" **ML models**, including architectures like EquiformerV2 and the latest methods topping material informatics benchmarks, has revealed a critical deficiency when applied to complex surfaces. These models often appear "unaware" of fundamental electronic phenomena, such as long-range charge redistribution or "charge sloshing" on surfaces, rendering them unreliable for surface chemistry and physics. This observation has solidified our conviction to move away from purely data-driven ML and towards methods with a stronger physical basis.

We have thus turned our attention to enhancing **semi-empirical** quantum mechanical methods, with a particular focus on **extended tight-binding (xTB)** approaches. We found that standard xTB parametrizations often lack accuracy for inorganic materials, which are central to quantum dots and many 2D systems. Even for organic components improvements can be substantial.

To address these shortcomings, we have explored several avenues. For organometallic molecules, we demonstrated that a **ΔML approach** can significantly improve the accuracy of xTB predictions. More powerfully, we have leveraged backpropagation through the XTB self-consistent field (SCF) procedure, as implemented in the dxtb package, to directly reparametrize elements.

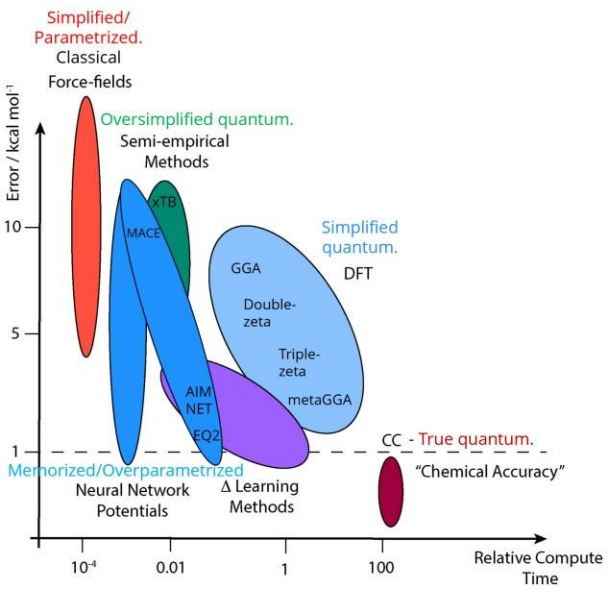


Fig. 1 Speed vs. accuracy of quantum computational methods

Our current research focuses on two synergistic paths: 1) Further accelerating physically-grounded methods like XTB, for instance, by developing ML models to provide superior **initial guesses for orbital charges**, thereby minimizing the number of SCF cycles. 2) Developing novel ML architectures that intrinsically incorporate physical principles, such as **electronegativity equilibration**, to ensure they can capture the long-range charge redistribution crucial for accurate surface and interface modeling.

This talk will present our findings, showcase specific examples from quantum dot surface chemistry and catalysis, and discuss the broader applicability of these hybrid and physically-informed accelerated methods to the quantum simulation of 2D materials, their heterostructures, and the devices they enable, offering valuable tools for the PQS2D and QTMND communities.

POSTER ABSTRACTS

Single-layer Triangular Graphene Quantum Dots with Nitrogen Impurity

S. Abedi, A. Wania Rodrigues, D. Miravet, and P. Hawrylak
University of Ottawa, Ontario K1A 0R6, Canada
sabed068@uottawa.ca

Triangular graphene quantum dots (TGQD) with zig-zag edges are synthetic structures in which the presence of a zero-energy shell at the Fermi level generates electronic correlations and entanglement [1–3]. The number of states in the zero-energy shell equals the imbalance between atoms in the two graphene sublattices, growing as the triangle increases in size. This allows us to generate a macroscopic, partially occupied shell, similar to the Lowest Landau level in the fractional quantum Hall effect. It also serves as a platform to design topological quantum matter with properties vastly different from its constituents, such as superconductivity and ferromagnetism.

We present here the result of tight-binding (TB) and density functional theory (DFT) calculations for [n]triangulene, a triangular quantum dot with broken sublattice symmetry, terminated through zig-zag edges. We observe that the number of zero-energy degenerate states increases linearly with the number of edge atoms as we consider various sizes for the triangulene structure. For TB calculations, we also consider tunnelling matrix elements covering up to 6th nearest neighbours and show that such treatment of TB approaches DFT for the zero-energy shell.

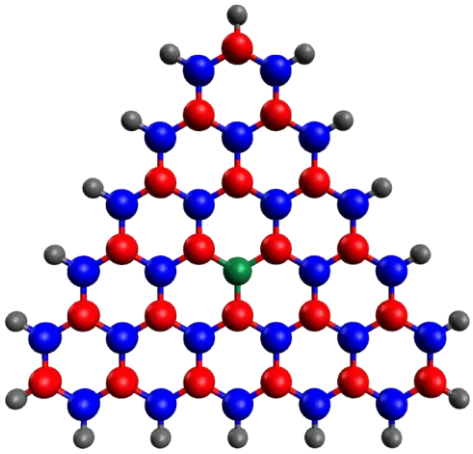


Fig. 1. [5]triangulene structure passivated with hydrogen atoms (grey dots). Red and blue dots correspond to sublattices A and B respectively. Green dot represents the nitrogen impurity.

We then introduce a localized impurity, replacing a carbon atom in the [n]triangulene with a single nitrogen atom. The localized nitrogen impurity introduces an extra positive charge and an electron into the system, thereby altering the total spin of the system [4, 5]. We compare the effects of the impurity positioned at the centre (shown in Fig 1) and off-centre. We demonstrate a shift in energy of the first state in the degenerate shell compared to the [n]triangulene with no impurity and the effect of the impurity on the wavefunction density of the zero energy states.

References

[1] A. D. Guclu, P. Potasz, O. Voznyy, M. Korkusinski & P. Hawrylak, Phys. Rev. Lett. **103**, 246805 (2009)
[2] A. D. Guclu, P. Potasz, M. Korkusinski & P. Hawrylak, “Graphene Quantum Dots”, Springer-Verlag (2014)
[3] A. D. Guclu, P. Potasz & P. Hawrylak Phys. Rev. B **84**, 035425 (2011)
[4] A. Wania Rodrigues, D. Miravet, J. Lawrence & P. Hawrylak, Solid State Communications **401**, 115899 (2025)
[5] J. Lawrence et al., ACS Nano **17**, 20237 (2023)

Tunable Artificial Superlattices in WSe_2 via Nanoscale Patterned Graphite Gates

A. M. Aygar[1,2], A. Luican-Mayer[1] and L. Gaudreau[2]
[1]*University of Ottawa, Ottawa, Ontario K1N 6N5, Canada*
[2]*National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada*
Melis.Aygar@uottawa.ca

The ability to simulate quantum many-body phenomena in solid-state systems has gained significant interest in recent years, with two-dimensional (2D) materials providing a versatile platform for such efforts. Recent studies have demonstrated that moiré superlattices formed by stacking TMD layers at small twist angles can host correlated electron states, enabling analog simulation of the Hubbard model [1–2]. However, this approach is limited by lack of dynamic tunability. Here, we propose employing a nanoscale patterned graphite gate to induce a periodic electrostatic potential in a monolayer of tungsten diselenide (WSe_2) creating an artificial superlattice. This approach offers dynamic tunability and design flexibility, providing a new pathway for quantum simulation in 2D materials.

The primary experimental challenge lies in the fabrication of the nanoscale periodic pattern on the graphite layer, which requires high-resolution techniques. We utilize electron beam lithography (EBL) to define sub-50 nm scale features on exfoliated graphite flakes, followed by reactive ion etching (RIE) to realize the periodic pattern. The processed graphite gate is then integrated into a van der Waals heterostructure through a deterministic dry transfer method, where monolayer WSe_2 is stacked on top of a thin hexagonal boron nitride (hBN) spacer, ensuring both cleanliness and proximity to the patterned gate for effective electrostatic coupling.

Characterization of the fabricated structures is essential to verify the pattern fidelity and surface quality. Scanning electron microscopy (SEM) is used to inspect the pattern geometry and uniformity, while atomic force microscopy (AFM) provides topographic maps of the etched features and ensures minimal damage to the surrounding material. These structural characterizations confirm the formation of well-defined periodic potentials at the nanoscale, which serve as the basis for the induced superlattice in the WSe_2 monolayer.

In future work, we will perform photoluminescence (PL) spectroscopy and low-temperature magnetotransport measurements to probe the resulting superlattice effects. PL measurements can reveal miniband formation, exciton localization, and potential modulation of the optical bandgap, while magnetotransport studies may exhibit features such as Hofstadter's butterfly, fractal energy spectra, or correlated insulating states. These experiments will help elucidate how tunable electrostatic superlattices affect quantum many-body interactions in 2D semiconductors, advancing the realization of analog quantum simulation platforms based on artificial lattices.

References

[1] Tang, Y., et al. Nature **579**, 353–358 (2020).
[2] Regan, E. C., et al. Nature **579**, 359–363 (2020).

Valley-Spin Polarization at Zero Magnetic Field Induced by Strong Hole-Hole Interactions in Monolayer WSe_2

J. Boddison-Chouinard[1,2], M. Korkusinski[1], A. Bogan[1], P. Barrios[1], P. Waldron[1], K. Watanabe[3], T. Taniguchi[3], J. Pawłowski[4], D. Miravet[2], P. Hawrylak[2], A. Luican-Mayer[2], and L. Gaudreau[1].
[1]*National Research Council Canada, Ottawa, Ontario, K1A 0R6, Canada*
[2]*University of Ottawa, Ottawa, Ontario, K1N 9A7, Canada*
[3]*National Institute for Materials Science, Tsukuba, Japan, 305-0044* [4]*Wrocław University of Science and Technology, Wrocław, Poland*
Justin.Boddison-Chouinard@nrc-cnrc.gc.ca

Monolayer transition metal dichalcogenides have emerged as key materials for investigating the intricate relationship between spin and valley degrees of freedom. The pronounced spin-orbit interaction and the lack of inversion symmetry in these materials result in a spin-valley locking effect, where carriers in the K and K' valleys of reciprocal space exhibit opposite spins based on which valley they reside. This effect is particularly pronounced for holes due to the larger spin-orbit gap in the valence band.

In this poster presentation, we demonstrate that by confining a monolayer of tungsten diselenide to one dimension via electrostatic confinement, the combination of the spin-valley locking mechanism and strong hole-hole interactions lead to a ferromagnetic state in which hole transport through the one-dimensional system is valley-spin polarized, even in the absence of an external magnetic field [1]. Furthermore, we demonstrate that the stability of the valley-spin polarized configuration can be tuned by a global back-gate. This observation opens the possibility of implementing a robust and stable valley polarized system, essential valleytronic applications.

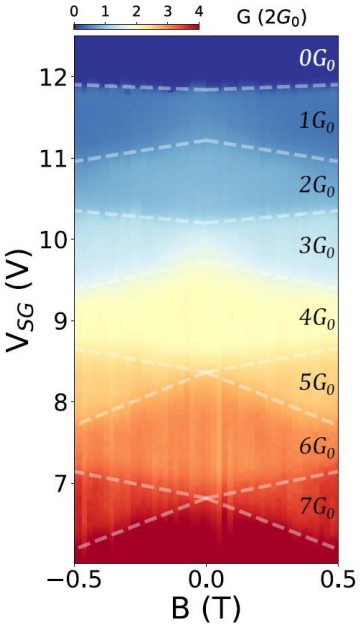


Fig. 1. Conductance as a function of the split gate voltage and magnetic field. Regions of constant conductance are outlined by dashed white lines.

References:

[1] J. Boddison-Chouinard, M. Korkusinski, A. Bogan, P. Barrios, P. Waldron, K. Watanabe, T. Taniguchi, J. Pawłowski, D. Miravet, P. Hawrylak, A. Luican-Mayer, and L. Gaudreau. *Valley-spin polarization at zero magnetic field induced by strong hole-hole interactions in monolayer WSe_2. arXiv:2410.11653* (2024).

New Polar Quantum Materials - Controlling Ferroelectricity and its Interaction with the Environment

J. Brunette[1], L. Molino[1], S. Chen[2], S. Walker[1], P. Grutter[2] and A. Luican-Mayer[1]
[1]Department of Physics, University of Ottawa, Ottawa, Canada [2]Department of physics, McGill University, Montréal, Canada
jbrun030@uottawa.ca

Twisting transition metal dichalcogenide (TMD) layers in the limit of very small angles, relaxes the moiré lattice into areas of energetically favorable stacking, creating a regime of triangular domains with alternating stacking of metal atoms aligned over chalcogen (MX), and chalcogens aligned over metal atoms (XM). Broken inversion symmetry in these domains leads to vertical polarization. Here, we explore the question of how this spatially varying polarization is influenced by and influences a proximal electrostatic environment. We show Scanning Tunneling Microscopy/Spectroscopy (STM/S) on graphene placed on top of marginally twisted WSe_2. In addition, using Kelvin Probe Force Microscopy (KPFM) we study how polarization depends on the substrate on which the marginally twisted layers are placed.

Bi-based bracelet-like monolayer with negative in-plane Poisson's ratio and enhanced photocatalytic performance: a first-principles study

N. Kedidi[1], T. Ayadi[2] and M. Debbichi[1]
Université de Monastir, Faculté des Sciences de Monastir, Laboratoire de la matière condensée et nanosciences LR11ES40, 5019 Monastir, Tunisia
Université Paris-Saclay, CEA, Service de recherche en Corrosion et Comportement des Matériaux, SRMP, 91191 Gif-sur-Yvette, France
Mourad.Debbichi@fsm.rnu.tn

Auxetic materials are in high demand for advanced applications due to their relatively rare negative Poisson's ratio in two-dimensional materials. This study investigates the structural, mechanical, electronic, optical and photocatalytic properties of the $AsBiTe_3$ monolayer (ML) using first-principles calculations. Through analysis of phonon dispersion curves, ab-initio molecular dynamics simulations, and Born conditions, we have confirmed the thermal, dynamic, and mechanical stability of the $AsBiTe_3$ monolayer. The study of the mechanical properties of this material revealed significant anisotropy and a bidirectional in-plane negative Poisson's ratio (NPR). In addition, electronic band structures calculated, with and without spin–orbit coupling (SOC) using the HSE functional, indicate that this monolayer exhibits the characteristics of an indirect-gap semiconductor around 1.17 and 1.32 eV, respectively. Notably, by assessing the optical properties of $AsBiTe_3$ monolayer, it has been found that this monolayer has a strong light-harvesting capability with an absorption coefficient higher than 10^5 cm $^{-1}$ in the visible region. Fascinatingly, under a biaxial 1% and 4% tensile and −2% compressive strain, the band edge of the $AsBiTe_3$ monolayer extends across the redox potential of water at pH = 0, 7 and 14, respectively. This suggests that this monolayer holds promise as a potential material for catalytic water splitting. These results should inspire further experimental and theoretical research, aimed at fully exploring the potential applications of this new class of 2D materials.

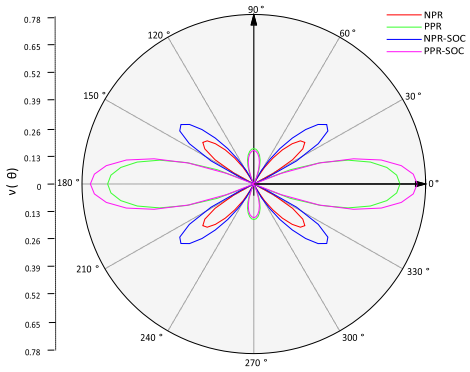


Fig.1 Poisson's ratio ν(θ) of $AsBiTe_3$ monolayer with and without spin orbital coupling (SOC) as a function of orientation.

References

[1] Kedidi, N., Ayadi, T., and Debbichi, M, J. Condens. Matter Phys. **36**, 205503 (2024).
[2] Kedidi, N., Ayadi, T., Debbichi, M., and Lebegue, S., ACS Applied Electronic Materials **5**, 5841 (2023).

Transport properties of the $LaNiO_2$ a DFT plus DMFT approach

Mijanur Islam[1], Sudipta Koley[2], and Saurabh Basu[1]
[1]*Department of Physics, Indian Institute of Technology-Guwahati, Guwahati 781039, India*
[2]*Department of Physics, Amity Institute of Applied Sciences, Amity University Kolkata, Kolkata 700135, India*
mijanurislam054@gmail.com

We study the transport properties of a nickelate $LaNiO_2$ compound using density functional theory (DFT) in conjunction with dynamical mean field theory (DMFT). An interacting multi-orbital spin-resolved scenario for $LaNiO_2$ yields a metallic ground state with ferromagnetic correlations. The latter contrasts with an antiferromagnetic order reported earlier. The metallic behavior persists even at large values of the interaction energies. Further support of the metallic state is provided by the angular resolved photoemission spectroscopy (ARPES) data.

References

[1] M. Islam, S. Koley, and S. Basu, Eur. Phys. J. B (2021) **94**:187.
[2] A.S. Botana, M.R. Norman, Phys. Rev. X **10**, 011024 (2020).

Fully Spin Polarized Hole Transport at Low Filling Factors in Monolayer WSe_2

Antoine Labbé[1,2], Justin Boddison-Chouinard[1,2], Alex Bogan[1], Pedro Barrios[1], Philip Waldron[1], Kenji Watanabe[3], Takashi Taniguchi[3], Adina Luican-Mayer[2], Louis Gaudreau[1]
[1] *National Research Council of Canada (Canada),*
[2] *University of Ottawa (Canada),*
[3] *National Institute of Material Science (Japan)*
alabb017@uottawa.ca, Louis.Gaudreau@nrc-cnrc.gc.ca, luican-mayer@uottawa.ca

One of the most promising and exciting family of two-dimensional (2D) materials is the semiconducting transition metal dichalcogenides (TMDs) [1]. Due to their 2D nature, charge carriers present in TMDs act as a 2D hole gas (2DHG) where applying a magnetic field leads to the Quantum Hall Effect [2]. Additionally, their lack of inversion symmetry at the monolayer limit and the presence of transition metals leads to opposite spins being locked to opposite valleys, also known as spin-valley locking, a phenomenon that can be leveraged for many quantum technologies [3]. Here, we introduce a device fabrication technique and architecture that enables the realization of low resistance ohmic contacts while maintaining a low carrier density in monolayer WSe_2 [4,5]. We then present magnetotransport measurements of this device and discuss the appearance of an unusual Landau fan diagram in which we observe fully spin polarized hole transport at low filling factors all the way to $\nu = 1$. We conclude by showing next generation devices that will allow greater tunability in the quantum Hall regime.

References:
[1] K. F. Mak, et al., Phy. Rev. Lett. **105**, 136805 (2010)
[2] R. Pisoni, (2019), Quantum transport in few-layer MoS2 [PhD thesis]
[3] X. Liu and M. C. Hersam, Nat. Rev. Matter. 669 (2019)
[4] J. Boddison-Chouinard, et al., npj 2D Mater. Appl. **7**, 50 (2023)
[5] J. Boddison-Chouinard, et al., Appl. Phys. Lett. **119**, 133104 (2021)

Exploring Alternative Layered Materials as Gate Dielectrics for 2D Material Based Devices

I. Lagaud[1,2], M. Aygar[1,2], A. Labbé[1,2], J. Boddison-Chouinard[1,2], Z. Sofer[3], Kenji Watanabe[4], Takashi Taniguchi[4], A. Luican-Mayer[1] and L. Gaudreau[2]
[1]*University of Ottawa, ON K1N 6N5, Canada*
[2]*National Research Council Canada, Ottawa, ON, K1A 0R6, Canada*
[3]*UCT Prague Department of Inorganic Chemistry, Prague Czech Republic*
[4]*National Institute of Material Science, Japan*
Ilaga008@uottawa.ca

The performance and scalability of 2D-based electronic devices are strongly influenced by the choice of gate dielectric. In transistor-based devices, high-κ dielectrics enhance electrostatic gate control, enabling faster switching speeds, increased device performance, and reduced gate leakage currents, an essential factor in extending the operational range. However, integrating conventional 3D high-κ dielectrics with 2D materials often results in poor interface quality, leading to high trap densities and reduced carrier mobility [1]. Hexagonal boron nitride (hBN), a 2D layered material, has become the standard gate dielectric in 2D heterostructures due to the clean interfaces it forms with other 2D materials. Nevertheless, its relatively low dielectric constant ($\kappa \approx 2.5 - 4$) [2] limits the operational range, as leakage currents become significant at higher gate voltages.

The project aims to explore alternative crystalline layered dielectrics, specifically LaOBr, LaOCl, and Bi_2SeO_5, that combine desirable properties such as high dielectric constants, large band gaps, and compatibility with van der Waals heterostructures. These materials offer promising potential to overcome the limitations of hBN while preserving the benefits of 2D-2D interfaces.

To evaluate these materials as gate dielectrics, we will fabricate encapsulated graphene Hall bar devices using the proposed layered dielectric. By measuring key electrical properties such as gate leakage current, carrier mobility, subthreshold slope, dielectric breakdown and the dielectric constant, we aim to directly assess their performance. This approach will establish a reliable benchmarking platform for evaluating crystalline dielectrics in 2Dbased devices.

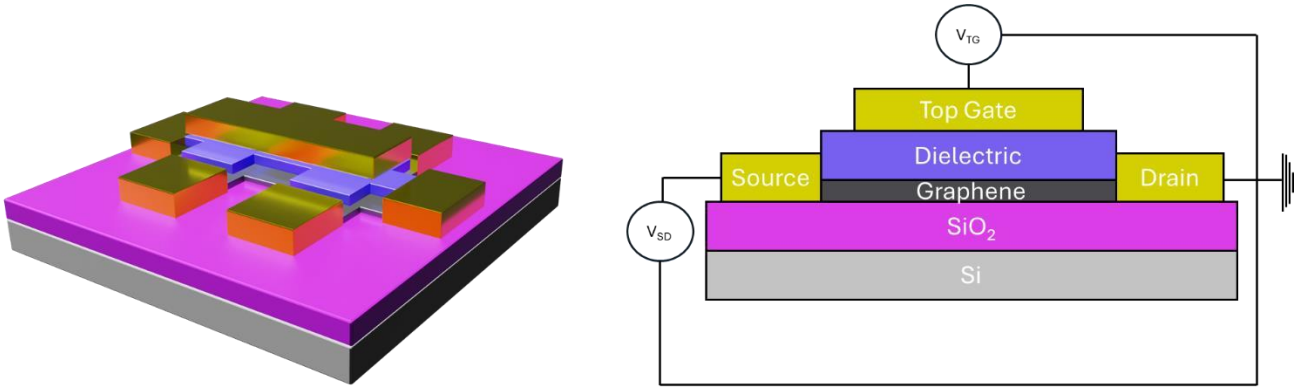


Fig. 1: Schematic of the device architecture

References:
[1] Illarionov, Y.Y., Knobloch, T., Jech, M. et al. *Insulators for 2D nanoelectronics: the gap to bridge.* Nat. Commun. **11**, 3385 (2020).
[2] Boddison-Chouinard, J., Bogan, A., Barrios, P. et al. *Anomalous conductance quantization of a one-dimensional channel in monolayer WSe_2.* npj 2D Mater Appl. **7**, 50 (2023).

Scanning Tunneling Microscopy of Twisted Multilayer Graphene

Xue-Ying LiYang[1], Sean M. Walker[1], Laurent Molino[1], Ryan Plumadore[1], Adina Luican-Mayer[1]
[1]*Department of Physics, University of Ottawa, Ottawa, Ontario, K2P 0W4, Canada*
xli584@uottawa.ca

Beyond twisted bilayer graphene, recent studies have proposed devices consisting of multiple graphene layers with near magic-angle twists, as a promising platform for experimentally realizing correlated topological states. Moiré superlattices originating from consecutive layers are expected to experience lattice relaxation that significantly modifies the electronic band structures [1].

Here, we present our progress in characterizing structural and electronic properties of a twisted multilayer graphene device using scanning probe microscopy, with focusing on regions of twisted mono-bilayer (1L+2L) featuring the existence of flat bands localized to rhombohedral stacked domains; helical trilayer regions (1L+1L+1L) and regions with two twisted layers twisted on top of Bernal bilayer (1L+1L+2L), forming various triangular domains that provide insight to how lattice relaxation modifies the electronic band structures.

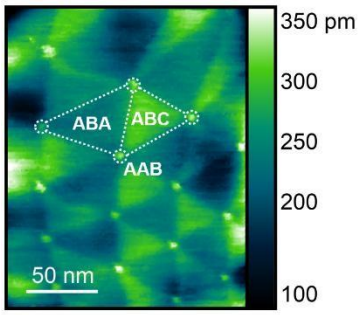


Fig. 1. STM topograph showing triangular reconstruction domains on twisted mono-bilayer (1L+2L) graphene.

References

[1] T. Devakul, Science **9**, No.36 (2023); J.Jang, arXiv: 2407.19143 (2024); Y.H. Kwan, Phys. Rev. B **109**, 125141 (2024); L. Xia, arXiv: 2310.12204 (2023); J.M. Park, Nature **590**, 249–255 (2021); Z. Hao, Science **371**, 1133–1138 (2021).

Development of a p-i-n avalanche photodiode based on WSe_2

Émile Roy[1,2,3], Sam Dehlavi[1,3] and Mathieu Massicotte[1,2,3 *]
[1]*Institut quantique, Université de Sherbrooke, QC, Canada*
[1]*Département de génie électrique et génie informatique, Université de Sherbrooke, QC, Canada*
[1]*Institut Interdisciplinaire d'Innovation Technologique (3IT),*
Laboratoire Nanotechnologies et Nanosystèmes
(LN2) - CNRS IRL-3463, QC, Canada
*Mathieu.Massicotte@usherbrooke.ca

The need for faster, more sensitive photodetectors continues to grow, particularly for optical telecommunications, laser remote sensing and medical imaging. Avalanche photodiodes (APDs) have set the standard for photodetection for over fifty years. Transition metal dichalcogenides (TMDs) have rapidly established themselves as a material of choice for the manufacture of optoelectronic devices with innovative properties. WSe_2 appears to be an excellent candidate for optical detector applications [1], thanks to its thickness-dependent direct bandgap and high amplification gain under the avalanche effect. This work investigates the avalanche mechanism in a WSe_2 based p-i-n junction by modifying the electric field profile. More precisely, this work focuses on the study of impact ionization coefficients, the key parameter of the avalanche mechanism [2], under the effect of the electric field in the p-i-n junction. We present in this work some preliminary results regarding the control of the avalanche mechanism. Studying the avalanche mechanism in WSe_2 could help to better direct the development of the next generation of optical detectors. In fact, investigating the potential of TMDs in APDs could open the door to the development of new SPADs.

[1] P. Martyniuk *et al.*, *Infrared avalanche photodiodes from bulk to 2D materials*, Light Sci Appl. **12**, 1, 212 (2023).
[2] Y. Okuto and C. R. Crowell, *Threshold energy effect on avalanche breakdown voltage in semiconductor junctions*, Solid-State Electronics **18**, 161-168 (1975).

InQuanto: Quantum chemistry on quantum computers

L. Szulakowska[1], C. Ward[1], G. Christopoulou[1], V. Bhasker[1], R. Anderson[1], O. Backhouse[1], R. Finsterhoelzl[1], D. Muñoz Ramo[1], A. Tranter [1], and InQuanto team[1]
[1]*Quantinuum, Terrington House, 13-15 Hills Road, Cambridge CB2 1NL, UK*
Ludmila.Szulakowska@quantinuum.com, Andrew.Tranter@quantinuum.com

Quantum chemistry methods have served as an essential tool for the simulation of molecules and materials across diverse industrial applications in chemistry, physics, biology, medicine, and beyond. Despite their crucial role in guiding design and property prediction, these methods are drastically constrained by the computational complexity of realistic models [1]. This limitation is particularly noticeable for strongly correlated systems, common in chemical reaction studies and the fields of magnetism and high-temperature superconductivity [1].

Quantum computing offers an attractive alternative for solving problems that have so far relied on density functional theory, coupled cluster methods, configuration-interaction-based approaches or other active space methods [1]. Some promising demonstrations of quantum computing for proof-of-concept calculations have been reported [1], although they are still primarily limited by hardware capabilities. To unlock the full potential of quantum computing applications, it is crucial to enable the transfer of knowledge between the field of quantum computing and quantum chemistry [1].

Quantinuum's InQuanto [2] is a Python-based quantum computational chemistry platform, crafted to facilitate quantum computational chemistry for researchers in industry and academia. InQuanto supports the complete quantum computational chemistry pipeline and includes a library of popular algorithms, such as variational quantum eigensolver (VQE) and variational quantum deflation (VQD), quantum subspace expansion (QSE) and quantum phase estimation (QPE). It includes a variety of ansatzes as well as backends from various providers. It offers a modular and backend-agnostic development ecosystem for quantum scientists to construct novel algorithms using building-block components for tailored chemistry applications.

We report here on how, working with partners, researchers at Quantinuum have used InQuanto with the world's highest performing ion-trap quantum hardware by Quantinuum to publish work exploring materials for carbon capture [3], investigating drug-protein binding mechanisms [4] and organic synthesis [5] as well as computing Green's functions for Fermi-Hubbard and impurity models [6].

References

[1] S. McArdle, S. Endo, A. Aspuru-Guzik, S. C. Benjamin, X. Yuan, Rev. Mod. Phys. **92**, 015003 (2020).
[2] InQuanto, 2025. URL https://www.quantinuum.com/products/inquanto.
[3] G. Greene-Diniz et al. EPJ Quantum Tech. **9**, 37 (2022).
[4] J. J. M. Kirsopp et al. Int. J. Quantum Chem. 122 (2022).
[5] G. Greene-Diniz et al. EPJ Quantum Tech. **9**, 37 (2022).
[6] G. Greene-Diniz et al. Quantum **8**, 1383 (2024).