International Workshop on Quantum Circuits in 2D Materials

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Contents

Thursday, 26/05

Opening session - 9:00am-9:30am, STEM 224
(*Chair: P. Hawrylak*)

1.1 Guy Levesque - uOttawa Associate Vice President, Research Support and Infrastructure

1.2 Louis Barriault - uOttawa Dean of Science

1.3 Julie Lefebvre, NRC Director General Security and Disruptive Technologies

Session 1 - 9:30am-10:30am, STEM 224
(*Chair: Y. Shim*)

2.1 Allan H. MacDonald

The Magic of Moiré Materials

A.H. MacDonald

Physics Department, University of Texas at Austin 78712 USA

Two-dimensional crystals that are overlaid with a difference in lattice constant or a relative twist form a moiré pattern. In semiconductors and semimetals, the low-energy electronic properties of these systems are described by Hamiltonians that have the periodicity of the moiré pattern, opening up a strategy to make artificial two-dimensional crystals with lattice constants on the ten nm scale. I refer to these artificial crystals as moiré materials. Because of their large lattice constants, the band filling factors of moiré materials can be tuned over large ranges without introducing chemical dopants simply by using electrical gates. Moiré materials, can be used to flexibly simulate the physics of real atomic scale crystals, and to create new states of matter. I will survey progress that has been made in understanding the low-temperature properties of the first moiré materials - twisted graphene systems in which electron velocities vanish at discrete magic angles and two-dimensional transition-metal dichalcogenide stacks that simulate atomic scale Hubbard model physics – and speculate on future directions.

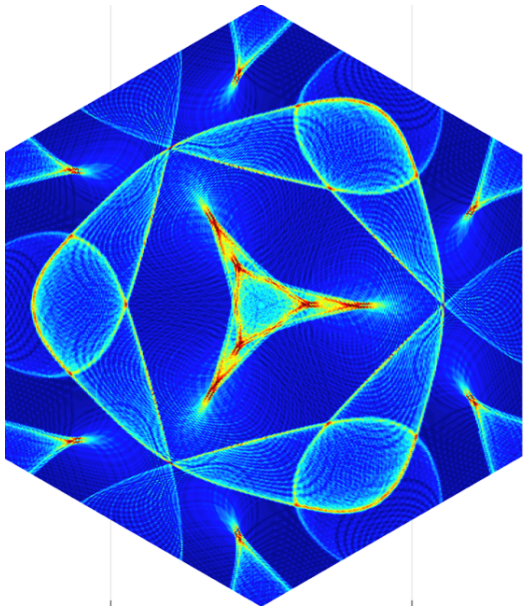

Figure 2.1: Heat-map for low-energy excitations of magic-angle twisted bilayer graphene as a function of momentum in the moiré Brillouin zone. Phase transitions between paramagnetic and ferromagnetic states are common in graphene moiré superlattice. From work in metals, it is known that these transitions are complicated by low-energy excitations of the Fermi sea, which give rise to non-analytic corrections to Fermi liquid theory. Moiré materials provide an excellent platform to study these transitions, among other fundamental aspects of the physics of interacting electrons in solids.

Many body enhanced spin-valley physics and light-matter couplings in hBN-MoS_2-hBN heterostructures

Jonathan Finley

Walter-Schottky-Institut and Physik Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

In this talk I will begin by exploring recent progress on magneto optical spectroscopy of atomically thin semiconductors with a special emphasis on the spin-valley physics of neutral and charged excitons. At charge neutrality, high field magneto-spectroscopy has revealed the g-factors and diamagnetic shifts of the exciton Rydberg states in the typical TMD monolayer semiconductors encapsulated in hBN [1,2]. In gated structures, tuned to provide excess electron or hole doping we examine the interaction of the exciton with the surrounding Fermi sea [3-5]. We observe spontaneous valley polarization of interacting Landau levels, reminiscent of magnetic phase transitions in hole doped WSe2 that arises due to enhanced Zeeman energies of carriers in interacting LLs. I will highlight our recent results on electron doped hBN encapsulated MoS_2, where we find that it is indeed the electron spin of the resident electron bath that defines the exciton spin and ground state of the dressed exciton [4,5]. Results cannot be understood within a single-particle picture, highlighting the importance of exchange interactions and intervalley correlations in determining the ground state of 2D excitons in monolayer semiconductors.

A second attractive feature of 2D materials is the ability to tailor their photo-physics by placing them onto nanopatterned, dielectrically engineered and photonic substrates. For $MoSe_2$ monolayers straddling Néel domain wall boundaries at the surface of periodically poled $LiNbO_3$, the very large in-plane electric fields ($\sim$ MV/cm) result in the formation of atomically abrupt 1D excitonic trapping potentials that may host novel correlated quantum states [6,7]. Finally, we turn our attention to hBN-MoS_2-hBN heterostructures coupled to Si_3N_4 nanobeam photonic cavities with Q>10000. Our approaches enhance the cavity field overlap with the 2D heterostructure, whilst preserving the integrity of the attached 2D heterostructure to allow excitons to move as they couple to the 0D-cavity mode. We observe a nonmonotonic temperature dependence of the cavity-trion interaction strength, consistent with the non-local mature of light-matter interactions [8]. Moreover, spatially resolved Raman spectroscopy reveals how excitons, lattice phonons and local nanomechanical vibrational modes couple to determine the resulting photo-physical response [8]. Our observations highlight the scope of atomically thin materials for novel device functionalities, as well as demonstrating how the complex interplay between different degrees of freedom inevitably determine their resulting photo-physics.

[1] A.V. Stier et al., Phys. Rev. Lett 120, 057405 (2018).
[2] M Goryca et al., Nature Comm. 10, 1 (2019).
[3] J. Li et al., Phys. Rev. Lett. 125, 147602 (2020).
[4] J. Klein et al., Phys. Rev. R. 3, L022009 (2021).
[5] J. Klein et al., Phys. Rev. B,105, L041302 (2022).
[6] P. Soubelet et al, Nano Lett. 21, 959-966, (2021).
[7] R. Ołdziejewski et al. ArXiv preprint arXiv:2106.07290 (2021).
[8] C. Qian et al., arXiv 2107.04387, (2021), arXiv 2202.10980, (2022) and C. Qian et al. 2204.04304v1 (2022).

Coffee break - 10:30am-11:00am

Session 2 - 11:00am-12:30am, STEM 224
(*Chair: J. Menard*)

4.1 Alexander W. Holleitner

Precisely positioned atomistic quantum emitters in monolayer MoS_2

Alexander W. Holleitner

Walter Schottky Institut and Physics Department, TU Munich, Germany

In this talk, I will demonstrate the deterministic generation of single defects acting as quantum emitters in monolayer MoS_2 van der Waals heterostructures. The emitters are naturally confined to the few atoms limit axially while having a lateral creation accuracy of ~9 nm generated by highly local helium ion irradiation only limited by secondary ion events [1-3]. We reach defect creation efficiencies close to unity in larger irradiated spots and as high as 18% for single shot irradiation. The optical line shape reveals a strong asymmetry resembling the interaction with LA/TA phonons. Employing the independent Boson model to our emission lines, we find that the emitters are spatially localized to a length scale of 2 nm, which is consistent with cryogenic scanning tunneling microscopy (STM) on the samples [3-5]. I will also discuss the level structure, the magnetic properties, and the absorption characteristics of the emitters [6]. The demonstrated methodology allows positioning single photon emitters with a precision of only a few nanometers in large arrays of quantum emitters [7] and in already stacked heterostructures with electrostatic gates [8]. Our work paves the way towards the controlled and deterministic generation of quantum emitters in monolayer transition metal dichalcogenides (TMDCs) van der Waals heterostructures as well as photonic, optoelectronic, and plasmonic quantum devices.

[1] J. Klein et al., Site-selectively generated photon emitters in monolayer MoS2 via local helium ion irradiation. Nature Comm. 10, 2755 (2019).
[2] J. Klein et al. Robust valley polarization of helium ion modified atomically thin MoS2, 2D Materials 5, 11007 (2018).
[3] E. Mitterreiter et al., Atomistic positioning of defects in helium ion treated single layer MoS2, Nano Letters 20, 4437 (2020)
[4] J. Klein, L. Sigl, et al., Engineering the luminescence and generation of individual defect emitters in atomically thin MoS2, ACS Photonics 8, 2, 669 (2021).
[5] E. Mitterreiter et al., The role of chalcogen vacancies for atomic defect emission in MoS2, Nature Communications 12, 3822 (2021).
[6] Hoïger et al. in preparation
[7] K. Barthelmi et al., Atomistic defects as single-photon emitters in atomically thin MoS2, APL Perspective 117, 070501 (2020).
[8] Hötger et al., Gate-switchable arrays of quantum light emitters in contacted monolayer MoS2 van der Waals heterodevices, Nano Letters 21, 1040 (2021).

4.2 Klaas-Jan Tielrooij

Hybrid erbium-graphene platform for quantum technologies

Klaas-Jan Tielrooij

Catalan Institute of Nanoscience and Nanotechnology (ICN2), BIST & CSIC, Bellaterra (Barcelona), 08193, Spain

Rare-earth ions, such as erbium Er^{3+}, are interesting building blocks for various quantum technologies, including computation, simulation, sensing, and quantum memories. They are characterized by ultralong coherence lifetimes and excellent optical addressability. Erbium furthermore plays an important role because it emits light at 1.5 microns – in the extensively used C-band of (classical) optical communication systems.

Recently [1], we have demonstrated a hybrid platform consisting of a nanolayer of erbium emitters (12 nm thick) and gate-tunable monolayer graphene, which combines the optical addressability of erbium ions with high-speed, all-electrical modulation of the strong nearfield interactions between the emitters and graphene. Modulation is made possible via both a p-doped silicon backgate and a polymer electrolyte topgate. In this hybrid erbium-graphene system, we observe a significant fraction of erbium ions with a decay rate that is enhanced by a factor 1,000 and higher, indicating extremely efficient emitter-graphene interaction: 99.9% of the energy of these excited erbium emitters flows to graphene. Furthermore, we actively and dynamically modulate the near-field interaction using moderate electrical signals (<10 V) that tune the Fermi energy of graphene. Specifically, the erbium-graphene interactions are dynamically modulated between the regime where the emitters lead to interband transitions in graphene, and the regime where they lead to excitation of intraband plasmons. Remarkably, we show modulation frequencies up to 300 kHz – many orders of magnitude faster than the intrinsic decay rate of erbium ions (75 Hz). The strong near-field interactions between erbium quantum emitters and graphene, and the fast all-electrical modulation of these near-field interactions is interesting, as previous nanophotonic systems could only achieve modulation mechanically or with intense optical pulses. Furthermore, it constitutes an enabling platform for integrated quantum technologies, for example opening routes to quantum entanglement generation by collective plasmon emission or photon emission with controlled waveform.

[1] D. Cano et al. Fast electrical modulation of strong near-field interactions between erbium emitters and graphene, Nat. Commun. 11, 4094 (2020)

Excitons and Phonons in 2D perovskites

Paulina Plochocka-Maude

Laboratoire National des Champs Magnetiques Intenses, CNRS-UJF-UPS-INSA, Toulouse, France
Department of Experimental Physics, Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology, Wroclaw, Poland

High environmental stability and surprisingly high efficiency of solar cells based on 2D perovskites have renewed interest in these materials. These natural quantum wells consist of planes of metal-halide octahedra, separated by organic spacers. Remarkably the organic spacers play crucial role in optoelectronic properties of these compounds. The characteristic for ionic crystal coupling of excitonic species to lattice vibration became particularly important in case of soft perovskite lattice. The nontrivial mutual dependencies between lattice dynamics, organic spacers and electronic excitation manifest in a complex absorption and emission spectrum which detailed origin is subject of ongoing controversy. First, I will discuss electronic properties of 2D perovskites with different thicknesses of the octahedral layers and two types of organic spacer. I will demonstrate that the energy spacing of excitonic features depends on organic spacer but very weakly depends on octahedral layer thickness. This indicates the vibrionic progression scenario which is confirmed by high magnetic fields studies up to 67T. Next, I will show that in 2D perovskites, the distortion imposed by the organic spacers governs the effective mass of the carriers. As a result, and unlike in any other semiconductor, the effective mass in 2D perovskites can be easily tailored. In the end, I will discuss exciton fine structure. The bright-dark splitting is also of paramount importance for light emitters which rely on the radiative recombination of excitons, since the excitons usually relax to the lowest lying dark state, which is detrimental for the device efficiency. I will discuss our optical spectroscopy measurements with an applied in-plane magnetic field to mix the bright and dark excitonic states of (PEA)2PbI4, providing the first direct measurement of the bright-dark splitting. The induced brightening of the dark state allows us to directly observe an enhancement of the absorption at the low-energy side of the spectrum related to the dark state. The evolution of the PL signal in the magnetic field, suggests that at low temperatures the exciton population is not fully thermalized due to the existence of a phonon bottleneck, which occurs due to the specific nature of the exciton-phonon coupling in soft perovskite materials.

Lunch break - 12:00am-2:00pm, Cafeteria Student Center

Session 3 - 2:00pm-3:20pm, STEM 224
(*Chair: F. Peeters*)

6.1 Pawel Potasz

Magnetic properties of moire quantum dot arrays

W. Pasek[1], **M. Kupczynski**[2], **P. Potasz**[1]

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[2]*Department of Theoretical Physics, Wroclaw University of Science and Technology, 50-370 Wroclaw, Poland*

New quantum simulators of Hubbard-like physics with high tunability of model parameters have been proposed in twisted transition metal dichalcogenide heterostructures [1,2]. Moire lattice constant can be controlled by the twist angle and the strength of a modulation potential by applying an external perpendicular electric field. We investigate magnetic properties of quantum dot arrays obtained from finite fragments of these moire superlattices. Starting from a reciprocal space model, we use the projection technique to obtain maximally localized Wannier functions and from them calculate generalized Hubbard model parameters [3,4]. We study how the relation between hopping integrals and interaction strength, and non-local interaction terms like interaction assisted hopping and direct exchange interaction affects the ground state properties [5]. Using exact diagonalization method, we show that high tunability of the model allows one to design nanostructures with nonzero total spin of the ground state in a wide range of filling factors. We propose that these ferromagnetic states can be switched on and off by applying an external perpendicular electric field. The results for different finite size systems are compared. Potential for designing Nagaoka ferromagnetism in moire quantum dot arrays is discussed.

[1] F. Wu, T. Lovorn, E. Tutuc, and A. H. MacDonald, Phys. Rev. Lett. 121, 026402 (2018).
[2] Y. Tang, et al., Nature 579, 353 (2020)..
[3] J. D. Cloizeaux, Phys. Rev. 135, A685, Phys. Rev. 135, A698 (1964).
[4] N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997).
[5] N. Morales-Durán, N. Hu, P. Potasz, A. H. MacDonald, arxiv:2108.03313 (2021).

6.2 Maciej Bieniek

Fine structure of neutral and charged excitons in monolayer MX_2 TMDs

M. Bieniek [1,2,3], **P. Hawrylak** [1]

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[2] *Department of Theoretical Physics, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*
[3] *Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*

We report here the effect of band nesting and topology on the fine structure of excitons and trions in the monolayer transition metal dichalcogenides (TMDs) family of 2D semiconductors. We start with an ab-initio based electronic structure obtained within a tight binding model of the MX_2 (M=Mo,W, X=S,Se,Te) family of direct gap semiconductors. We next turn on electron-electron interactions, form a Hartree-Fock ground state, and construct electron-hole excitations. We compute electron-electron interactions, self-energy in the screened exchange and Coulomb hole approximation and direct and exchange electron-hole interaction. We solve the Bethe-Salpeter equation to obtain a highly converged spectrum of exciton states. We disentangle effects of electron-hole dispersion, details of band structure on Coulomb intra/inter - valley interactions, topology of wavefunctions, screening and dielectric environment. In particular, we discuss the effect of SU(3) symmetric Q points and band nesting on ground and excited states of excitons. By the precise inclusion of spin splitting in our calculations, we establish the splitting between dark and bright exciton species. Next, motivated by recent experiments, we propose novel intra- and inter-valley singlet trions, constituting the trion fine structure distinct from that already known in bright and dark 2D materials with large conduction-band splitting induced by the spin-orbit coupling. We show that the trion energy splitting in MX2 is a sensitive probe of inter- and intra-valley carrier interaction.

From quantum dots to dopants in silicon

Michał Zieliński

Nicolaus Copernicus University, Toruń, Poland

We discuss our recent progress in atomistic modeling of a broad range of nanostructures. We start with alloyed quantum dots and inspect the role of alloy randomness that triggers the optical activity of dark excitons. Next, for 2D-like nanostructures with no alloying – so-called crystal phase quantum dots – we show that coupling between two sections of wurtzite leads to the formation of quasi-molecular hole states that may have an unusual antibonding character. Last but not least, we demonstrate that the same computational tools can be used to simulate STM images of dopants in silicon.

6.4 Oleksandr Voznyy

Exciton fine structure of CsPbBr3 perovskite quantum dots, a first-principles study

Oleksandr Voznyy, Kamalpreet Singh

University of Toronto Scarborough, 1265 Military Trail, Scarborough, ON M1C 1A4

Cesium lead halide perovskite nanocrystals are a highly attractive class of materials for coherent light emission, with implications for lasing, light-emitting diodes, and quantum computing. Fine-tuning their properties for the above applications requires an exact understanding of their exciton fine structure, in particular, spacing and polarization of their triplet and singlet states.

Experimental reports have been controversial, implicating that the Rashba effect may be inducing an inversion in the order of bright and dark states.

To aid in the resolution of this debate, we performed investigation of the fine structure of the triplet emission properties in these materials. Using the wave functions generated via DFT calculations including spin-orbit coupling for cubic, orthorhombic and tetragonal caesium lead halide perovskite nanocrystals of 3 nm in diameter, we further augmented them with Coulomb coupling between the exciton configurations, to resolve the absorption and emission fine structure in a configuration interaction method.

We anticipate our work will aid in the resolution of the debated emission fine structure of CsPbBr3 nanocrystals and thereafter allow for the development of bright materials for optoelectronics.

Coffee break - 3:20pm-3:40pm

Shot gun & poster session - 3:40pm-5:00pm
(*Chair: J. Menard*)

8.1 Nicolas Couture

8.2 Ilhem Bargaoui

8.3 Ahmed Jaber

8.4 Défi Junior Jubgang Fandio

8.5 Ryan Plumadore

8.6 Yasser Saleem

8.7 David Gayowsky

8.8 Ludmila Szulakowska

8.9 Maciej Bieniek

8.10 Alina Wania Rodrigues

8.11 Katarzyna Sadecka

8.12 Abdulmenaf Altintaş

8.13 Megan Cowie

8.14 Benjamin Puzantian

8.15 Laurent Molino

8.16 Jacob Manalo

ARC and STEM building lab tour - 5:00pm-7:00pm

Friday, 27/05
Session 4 - 9:00am-10:30am, STEM 224
(*Chair: A. Sachrajda*)

10.1 François Peeters

Deformed graphene

François Peeters

Physics Department, Universiteit Antwerpen, 2020 Antwerpen, Belgium

Two dimensional atomic thin materials can withstand enormous strains. This gives birth to a new area in physics where the properties of materials can be tuned without having to change its chemical composition. Such strains can be applied externally or be induced through the interaction with a substrate. Nanostructuring the substrate allows for specific patterns of deformation and consequently non-uniform strain fields. Periodic buckling of graphene has been shown recently to be able to restructure the energy spectrum of charge carriers into flat bands.

Strained graphene presents itself as a complementary platform to twisted graphene layers as a playground for new physics, from exotic topological quantum phases, to analogies with other fields (from quantum electrodynamics to quantum gravity), and even connects with traditional arts like origami and kirigami.

Nanobubbles can be fabricated with radius down to sub-nanometer allowing to investigate graphene under ultra-high strain. These nanobubbles can be filled with gasses and liquids which leads to novel physics of nanoconfined materials under high pressure.

Quantum devices in graphene

Klaus Ensslin

ETH, Zurich, Switzerland

Graphene and other 2D materials offer a huge potential for the realization of quantum devices. We demonstrate single shot read-out in bilayer graphene quantum dots and measure T_1 times of up to 50 ms for the spin excited state. In magic-angle twisted bilayer graphene we realize a SQUID and tune to both asymmetric and symmetric SQUID configurations by electrostatically controlling the critical currents through the junctions. We discuss further prospects of quantum devices in graphene.

10.3 Ke Wang

Manipulating Electrons in Gate-defined van der Waals Nanostructures.

Ke Wang

Department of Physics, University of Minnesota, USA

Since the discovery of graphene via mechanical exfoliation, it has been shown that the electronic properties of solids can undergo dramatic change when the material thickness is reduced to the atomic limit. Their exotic bandstructures are uniquely different from those in conventional 2DEGs. In particular, the broken inversion symmetry and strong spin-orbit interaction in semiconducting transition metal dichalcogenides (TMDs) polarizes spins in the opposite direction near the band edges of each valley, providing unique opportunity for novel spin and valley-based electronics. The relativistic charge carriers in monolayer graphene can be manipulated in manners akin to conventional optics, leading to electronic device concepts analogous to optical circuits (electron-optics). In this talk, we will discuss about novel gate-defined nanostructures in graphene and TMD, which recently allowed us to demonstrate controlled electron-optic interference process at zero magnetic field as a consequence of consecutive Veselago refractions in graphene microcavity, and and electrostatic confinement and tunable life-time of optical-trions in a TMD quantum dot.

[1] Gate-tunable Veselago Interference in a Bipolar Graphene Microcavity, Xi Zhang*, Wei Ren*, Elliot Bell, Ziyan Zhu, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras, Mitchell Luskin, Ke Wang, ArXiv: 2106.09651 (2021).
[2] Electrical Control of Charged Carriers and Excitons in Atomically Thin Materials, K. Wang, K. D. Greve, L. A. Jauregui, A. Sushko, A. High, Y. Zhou, G. Scuri, T. Taniguchi, K. Watanabe, M. D. Lukin, H. Park, P. Kim. Nature Nanotechnology 13, 128–132 (2018).

Coffee break - 10:30am-11:00am

Session 5 - 11:00am-12:30am, STEM 224
(*Chair: L. Gaudreau*)

12.1 Hugh Churchill

Toward valley-spin and gatemon qubits with 2D semiconductors and insulators

Hugh Churchill

University of Arkansas, USA

In this talk I will describe various collaborative efforts between my lab and others to create novel qubits that take advantage of the properties 2D semiconductors and insulators. First, I will discuss our progress in the fabrication and characterization of ambipolar double quantum dots in monolayer and bilayer WSe2, which I will argue is a compelling platform for the realization of valley-spin qubits. Next, I will summarize our work investigating hBN as a high-performance gate dielectric for Al/InAs Josephson junctions, which will be used for gatemon qubits. The third example is superconductor/semiconductor devices based on Ge quantum wells with epitaxial Al, also intended for gatemons. Finally, I will describe the MonArk NSF Quantum Foundry, a recently launched center jointly operated by the University of Arkansas and Montana State University that seeks to rapidly accelerate the fabrication and characterization of 2D quantum materials and devices.

12.2 Christoph Stampfer

On the spin and valley degree of freedom in bilayer graphene quantum devices

Christoph Stampfer

JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany

Graphene and bilayer graphene (BLG) are attractive platforms for quantum circuits. This has motivated substantial efforts in studying quantum dot (QD) devices based on graphene and BLG. The major challenge in this context is the missing band-gap in graphene, which does not allow to confine electrons by means of electrostatics. A widely used approach to tackle this problem was to introduce a hard-wall confinement by etching the graphene sheet. However, the influence of edge disorder, turned out to be a roadblock for obtaining clean quantum devices. The problem of edge disorder can be circumvented in clean BLG, thanks to the fact that this material offers a tunable band-gap in the presence of a perpendicularly applied electric field, a feature that allows introducing electrostatic soft confinement in BLG.

Here we present gate-controlled single, double, and triple dot operation in electrostatically gaped BLG. We show a remarkable degree of control of our devices, which allows the implementation of gate-defined electron-hole and electron-electron double-dot systems, where single-electron occupation becomes possible. Also in the single dot regime, we reach the very few electron/hole regime, extract excited state energies and investigate their evolution in a parallel and perpendicular magnetic field. Finally, we will show data on ultra-clean BLG quantum point contacts allowing investigating the spin-valley coupling in bilayer graphene.

12.3 Adam W. Tsen

Vertical van der Waals Heterostructures for Photosensing and Photocurrent Imaging

Adam W Tsen

Institute for Quantum Computing, University of Waterloo, Waterloo, Canada

I will discuss our recent work interfacing transition metal dichalcogenides with other 2D materials in vertical device geometries for broadband light sensing and photocurrent imaging of metal-insulator transitions. Specifically, we engineer graphene/2H-$MoTe_2$/black phosphorus photodetectors that are highly sensitive to photon energies continuously between the mid-infrared to deep-ultraviolet with large electrical bandwidth. The devices can be further utilized to perform local broadband absorption spectroscopy beyond the diffraction limit. On 1T-TaS_2/WSe_2/graphene heterostructures, we use photocurrent microscopy to spatially map the nearly commensurate (metal) to commensurate (insulator) charge density wave transition in 2D 1T-TaS_2 driven by both temperature and electric field.

Lunch break - 12:00am-2:00pm, Cafeteria Student Center

Session 6 - 2:00pm-3:20pm, STEM 224
(*Chair: P.Potasz*)

14.1 Justin Boddison-Chouinard

Transport in Quantum Confined 2D Semiconductors

Justin Boddison-Chouinard

Department of Physics, University of Ottawa, Ottawa, Canada

Quantum confinement in two-dimensional (2D) transition metal dichalcogenides (TMDs) offers the opportunity to create unique quantum states that can be practical for quantum technologies. The interplay between charge carrier spin and valley, as well as the possibility to address their quantum states electrically and optically, makes 2D TMDs an emerging platform for the development of quantum devices.

In this talk, we present the fabrication of a fully encapsulated monolayer tungsten diselenide (WSe_2) based device in which we realize gate-controlled hole quantum dots. We demonstrate how our device architecture allows us to identify and control the quantum dots formed in the local minima of electrostatic potential fluctuations in the WSe2 using gates. Coulomb blockade peaks and diamonds are observed which allow us to extract information about the dot diameter and its charging energy. Furthermore, we demonstrate how the transport passing through the channel formed by two gates is sensitive to the occupation of a nearby quantum dot. Additionally, we show how this channel can be tuned to be in the charge detection or the Coulomb blockade regime. Finally, we present a new device architecture which exhibits quantized conductance plateaus over a channel length of 600 nm at a temperature of 4 K. Quantized conductance over such a long channel provides an opportunity to incorporate gate defined quantum dot circuits without the nuisance of inhomogeneity within the channel.

14.2 Ludmila Szulakowska

Valley- and spin-polarized broken-symmetry states of interacting electrons in gated MoS_2 quantum dots

L. Szulakowska[1,3], M. Cygorek[1,5], M.Bieniek[1,2,4], P. Hawrylak[1]

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The realization of electron spin and valley qubits and quantum circuits in 2D materials requires control over electron numbers and understanding and control of interacting electron phases. Due to the reduced screening, atomically thin 2D materials offer an excellent platform to host strongly interacting electrons, which can be controlled in these materials with external confining potential [1,2,3,4]. Varieties of phases of matter arise, as the strong interactions interplay with valley degree of freedom on hexagonal lattice and with strong spin-orbit coupling of transition-metal-based crystals [4-10].

In this work, we show how strongly interacting electrons in monolayer transition metal dichalcogenide MoS2 can be tuned by metallic gates placed on top of the 2D crystal forming a parabolic quantum dot confinement [6,7,9]. The single particle energy structure a parabolic MoS2 quantum dot consists of twofold valley-degenerate quantum harmonic oscillator ladder of states originating in K and K' valleys as well as a sixfold degenerate spectrum derived from Q and Q'-points, with shell splitting arising due to valley-contrasting Berry curvature [9]. We populate these single particle energy states with up to six interacting electrons and use exact diagonalization to obtain the ground state as a function of the confining potential shell spacing ω [10].

We predict the formation of two types of broken symmetry states tunable by ω : both spin and valley polarized state for small ω and valley unpolarised but spin intervalley antiferromagnetic phase for large ω. This behavior is explained as a combined effect of the strong SO splitting, weak intervalley exchange interaction and strong correlations [10]. We propose how to detect these distinct phases in a spin valley blockade experiment [10].

[1] M. Korkusinski, W. Sheng, P. Hawrylak, Designing quantum systems in self-assembled quantum dots, *Phys. Status Solidi B* 238, 246 (2003).

[2] X.-X. Song, D. Liu, V. Mosallanejad, J. You, T.-Y. Han, D.-T. Chen, H.-O. Li, G. Cao, M. Xiao, G.-C. Guo, G.-P. Guo, A gate defined quantum dot on the two-dimensional transition metal dichalcogenide semiconductor WSe2, *Nanoscale* 7, 16867 (2015).

[3] Justin Boddison-Chouinard, Alex Bogan, Norman Fong, Kenji Watanabe, Takashi Taniguchi, Abdulmenaf Altintas, Maciej Bieniek, Pawel Hawrylak, Adina Luican-Mayer, and Louis Gaudreau, Gate controlled quantum dots in monolayer WSe2 , *Appl. Phys. Lett.* 119, 133104 (2021).

[4] K. F. Mak, C. Lee, J. Hone, J. Shan, T. F. Heinz, Atomically Thin MoS2: A New Direct-Gap Semiconductor, *Phys. Rev. Lett.* 105, 136805 (2010).

[5] E. S. Kadantsev P. Hawrylak, Electronic structure of a single MoS2 monolayer, *Solid St. Comm.* 152, 909 (2012).

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14.3 Marek Korkusinski

Spontaneous valley and spin symmetry broken states of interacting electrons in gated bilayer graphene quantum dots

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Bilayer graphene (BG) is a two-dimensional material with properties placing it between the monolayer graphene (MG) and monolayer transition-metal dichalcogenides (TDMCs). The MG exhibits a zero bandgap and supports massless Dirac Fermions, making it impossible to create a gate-defined confining potentials for carriers [1]. Graphene quantum dots (QDs) are created in the form of clusters of carbon atoms which, with the appropriate choice of the edge type, support a band of zero-energy edge states [2]. By filling these states with electrons, it is possible to design a quantum system with tailored magnetic and optical properties as a function of QD size and electron number [3]. By contrast, the TDMCs exhibit a wide bandgap and support massive Dirac Fermions, making it possible to confine the carriers with a potential created by gates [4]. The TMDC QDs are extensively studied as candidates for electron spin and valley qubits and quantum circuits in 2D [5]. However, owing to strong Coulomb interactions, the valley degree of freedom, and strong spin-orbit interactions, the electrons confined in TDMC QDs can form complex phases of different spin and valley polarizations [6].

Like MG, BG is a zero-bandgap system, but the Fermions propagating in it are massive. Moreover, the bandgap can be opened by applying an electric field normal to the layers [7,8]. Similarly to TDMCs, the physics of carriers is dominated by valley effect, but the spin-orbit interaction is too weak to create the spin-valley locking [8]. As a result, electrons or electron-hole pairs can be confined in BG QDs and their properties can be broadly tuned electrostatically [9].

In this work, we consider a BG QD with a gate-induced confinement potential [10]. We calculate the potential profile accounting for the BG band electrons self-consistently. The single-particle states of confined carriers, calculated using an atomistic tight-binding model, reveal the valley- and spin-degenerate ladder of states originating in the K and K' valleys. We populate these states with up to six interacting electrons and calculate their ground states as a function of the strength of the confinement and of Coulomb interactions using the exact diagonalization approach. We map out the spin and valley phase diagram and find that in the strong interaction regime the electrons form spin- and valley-polarized phases, whilst for a weak interaction strength the carriers occupy both valleys in a low total spin configuration. When the system is tuned from one regime to the other, the electrons redistribute through a series of spin and valley phase transitions. This behavior is explained as a result of an interplay of strong intra-valley exchange and correlations in the absence of inter-valley exchange

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14.4 Yun-Pil Shim

Creating excitons with structured light in transition metal dichalcogenides

Yun-Pil Shim

The University of Texas at El Paso

Recent progress in two-dimensional transition metal dichalcogenide (TMDC) has demonstrated that this family of materials is promising for applications in electronics, photonics, spintronics, and quantum information. Light has been one of the main tools to control and study the physical properties of TMDCs. Typical light sources can create excitons with particular spin states involving specific valleys due to the spin-valley locking. In addition to these bright excitons, a structured light beam such as a vortex beam can create dark excitons because of the nonzero orbital angular momentum of the light. It can potentially lead to an interesting system where one can study new strongly-correlated phenomena of the long-lived dark excitons. Using an effective two-band model coupled to structured light beams, we present theoretical results on the interplay between the light and the various excitonic excitations in monolayer TMDC materials.

Coffee break - 3:20pm-3:40pm

Session 7 - 3:40pm-5:00pm, STEM 224
(*Chair: M. Zielinski*)

16.1 Juan Ignacio Climente Plasencia

Metal chalcogenide colloidal nanoplatelets - insights from effective mass theory

Juan Ignacio Climente Plasencia

Universidad Jaume 2, Castellan, Spain

Semiconductor colloidal nanoplatelets are quasi-2D nanocrystals, which are often considered to be the wet chemistry analogous of epitaxial quantum wells. They show however a few distinct features that lead to characteristic properties: (i) the presence of weak, but finite lateral confinement; (ii) the presence of strong dielectric confinement posed by organic ligands surrounding the inorganic platelets; (iii) the possibility of building radial heterostructures.

In this presentation we give an overview on our group's attempts to provide insight into the photophysics of these systems using effective mass Hamiltonians. The electronic structure of CdSe-based nanoplatelets (homo and heterostructures) is reported for excitons, charged excitons and biexcitons. It is found that Coulomb interactions, boosted by dielectric confinement, play a prominent role in determining the physical response of these systems.

Overview of the D-Wave Advantage technology

Gabriel Poulin-Lamarre

D-wave, Burnaby, BC, Canada

D-Wave is the only quantum computing company providing commercial solutions based on annealing quantum computing: a heuristic well suited for tackling optimization, machine learning, and quantum system simulation problems. In the Advantage technology release, D-Wave has focused on increasing both the number of qubits and the graph connectivity, thus offering the possibility to solve larger problems. In this presentation, I will provide an overview of the recent changes and present high level results showing how the new technology performs against the previous 2000 qubit generation.

16.3 Udson Mendez

CMC Microsystems: Democratizing Access to Quantum Technologies

Udson Mendes

CMC Microsystems, Sherbrooke, QC, Canada

CMC's mission is to democratize access to state-of-the-art quantum hardware and software technologies to different sectors of Canada's quantum ecosystem. In this talk, I will give a brief overview of CMC's quantum computing services offered to Canadian academics, Startup's and industrial clients. These services include access to CAD tools, fabrication of superconducting, CMOS and photonics devices, access to quantum computing systems and training of highly-qualified personnel.

Invited speakers dinner - 6:00pm-8:00pm, 1st Elgin NAC

Saturday, 28/05
Session 8 - 9:30am-10:30am, STEM 224
(*Chair: A. Luican-Mayer*)

18.1 A.D. Güçlü

Quantum Monte Carlo study of semiconductor artificial graphene quantum dots

A.D. Güçlü

Izmir Institute of Technology, Dept. of Physics, 35430, Izmir, Turkey

Engineering graphene at the nanoscale introduces dramatic changes in the low energy spectrum due to broken sublattice symmetry: a tunable energy gap and magnetic zero-energy modes appear, making graphene nanostructures ideal candidates for nanoelectronic and spintronic applications[1]. While it is difficult to manipulate graphene structures at the atomic scale to reach desired properties, semiconductor artificial graphene can offer better controllability and thus play an important role in honeycomb lattice based nanoelectronics device design [2-3]. In this work, we performed variational and diffusion quantum Monte Carlo (QMC) calculations to take into account correlation and magnetic effects in hexagonal and triangular artificial graphene nanostructures[4]. I will show that QMC calculations using various many-body trial wave functions built from tight-binding, mean-field Hubbard and localized orbitals, allow us to accurately unveil metallic and antiferromagnetic phases in terms of dot-to-dot length, quantum well width and depth, as well as finite size effects.

This work was supported by The Scientific and Technological Research Council of Turkey (TUBITAK) under the 1001 Grant Project Number 119F119.

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Single electron spectroscopy and ultrafast time resolution by AFM

Peter Grutter

Department of Physics, McGill University, Montréal, Canada

It is well-established that Atomic Force Microscopy (AFM) can determine the atomic structure of surfaces and molecules. I will give an overview of some of our current research aimed at mechanically detecting single electrons, allowing us to perform electron energy spectroscopy of a single molecule on a metallic electrode interface. I will briefly touch on our current project to adapt this method to detecting individual ionized dopant atoms and their quantum mechanical coupling. As a second topic I will discuss our recent achievement in measuring opto-electronic properties with ultrafast temporal resolution by combining fs lasers with UHV AFM. This opens the door to understanding charge dynamics at the relevant fundamental time and length scale on surfaces or in molecules, and in particular the role of defects.

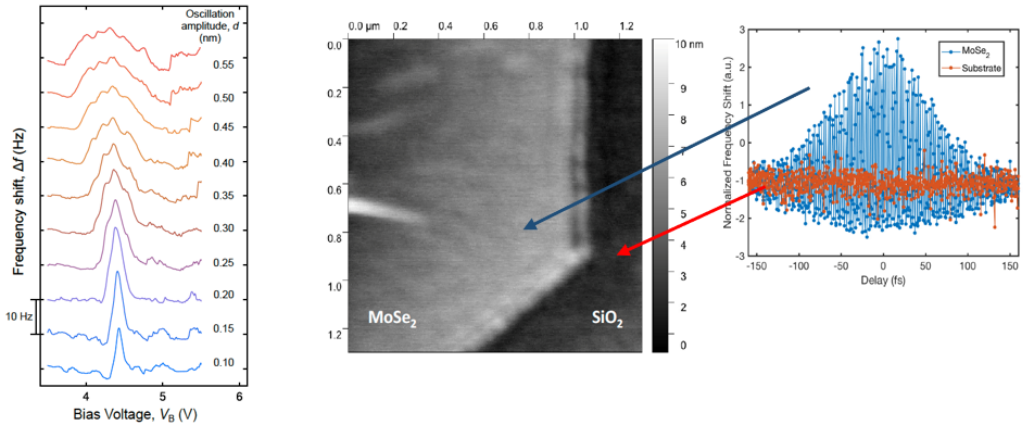

Figure 18.1: Left image: AFM Frequency shift spectra, with increasing force sensor oscillation amplitude (i.e. coupling strength), measured 10 nm above a single ferrocene molecule at 4.8 K. From this data one can directly deduce (without assumptions) the molecular reorganization energy, nuclear-electron coupling constants and molecular vibration frequencies. [Nano Lett. 19, 6104 (2019].
Right image: Optical autocorrelation function measured by AFM with spatial resolution on $MoSe_2$. [Proc. Natl. Acad. Sci. USA 117, 19773 (2020)]

Coffee break - 10:30am-11:00am

Session 9 - 11:00am-12:30am, STEM 224
(*Chair: J. Gupta*)

20.1 Ziliang Ye

Spontaneous polarization induced photovoltaic effects in Van der Waals semiconductors

Ziliang Ye

Department of Physics and Astronomy, Quantum Matter Institute, University of British Columbia, Vancouver BC, Canada

Conventional photovoltaic effects result from the drift of optically excited carriers under a built-in electric field, which is induced either by inhomogeneous doping or by interfacing materials of different work functions. On the other hand, a PV effect can also arise in a homogenous single crystalline material with low symmetry in a phenomenon so called bulk photovoltaic effect. Recently we observed a bulk photovoltaic effect in a semiconducting MoS_2 with rhombohedral stacking. The effect is enabled by an out-of-plane spontaneous polarization emerging from the unusual stacking order. Compared with conventional PV effects, the 3R MoS_2 based device has a similar quantum efficiency with a high speed and potentially a programmable polarity. Such rhombohedral stacked transition metal dichalcogenides provide a new platform for studying BPV and ferroelectricity at the atomically thin limit.

20.2 Simonas Krotkus

Wafer-scale (MO)CVD synthesis of two-dimensional materials and their heterostructures

S.Krotkus[1], S. Pasko[1], M.Heuken[1], X. Wang[2], B. Conran[2], C. McAleese[2], O.Whear[2]

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Due to their unique physical properties two-dimensional (2D) materials have attracted interest from a wide range of fields [1-4]. Moreover, the van der Waals bonding between individual 2D films allows to combine conducting, semiconducting and insulating 2D materials without the restraint of crystal lattice matching [5-7]. While exfoliated 2D films have been used extensively to show proof-of-concept of various device applications, technically delicate transfer processes render such approach hard to scale up. On the other hand, metal-organic chemical vapor deposition (MOCVD) enables synthesis of 2D materials on the wafer scale, as well as provide a route for 2D heterostructures with well-defined interfaces. Thus, MOCVD is highly reliable industrial deposition method for 2D materials, especially when volume production is considered.

In this talk, we present growth study of transition-metal dichalcogenides (TMDCs), e.g., molybdenum disulfide (MoS_2) or tungsten disulfide (WS_2), as well as graphene and hexagonal boron nitride (h-BN) on single-crystalline C-plane (0001) sapphire deposited in commercial AIXTRON reactors. Molybdenum hexacarbonyl, tungsten hexacarbonyl and di-tert-butyl sulfide are employed as metal-organic precursors for TMDC synthesis, while high temperature CVD-route using methane and borazine precursors is explored for graphene and h-BN, respectively. Crystal quality and epitaxial relationships of resulting 2D films is corroborated by number of microscopic and spectroscopic techniques, such as SEM, AFM, Raman and XPS. Finally, number of proof-of-concept devices based on (MO)CVD deposited 2D layers and their heterostructures will be presented.

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Epitaxial growth of transition metal dichalcogenide monolayers and heterostructures for large area device applications

Joan Redwing

Department of Materials Science and Engineering and 2D Crystal Consortium Materials Innovation Platform, The Pennsylvania State University, University Park, PA 16802

Wafer-scale epitaxial growth of semiconducting transition metal dichalcogenide (TMD) monolayers such as MoS_2, WS_2 and WSe_2 is of significant interest for device applications to circumvent size limitations associated with the use of exfoliated flakes. Epitaxy is required to achieve single crystal films over large areas via coalescence of TMD domains with the same crystallographic direction.

In this talk, I will discuss the prospects and challenges associated with the epitaxial growth of wafer-scale TMD monolayers and heterostructures for the development of large area 2D devices. Metalorganic chemical vapor deposition (MOCVD) has emerged as an enabling growth technology for TMDs due to its ability to achieve a combination of high growth temperatures (>700°C) and large chalcogen overpressures which are needed to obtain stoichiometric epitaxial films. The unique aspects of van der Waals epitaxy of TMDs on c-plane sapphire substrates will be presented including the role of surface passivation and steps on domain alignment and defects. Techniques for wafer-scale 2D layer transfer for device integration will be reviewed and applications for wafer-scale TMD monolayers in nanoelectronics, sensing and photonics will be presented.

Lunch break - 12:00am-2:00pm, Cafeteria Student Center

NRC lab tour - 2:00pm-3:20pm

Compact and portable THz time-domain spectrometer

Nicolas Couture, Akif Ahmed, Mamoun Wahbeh, Garland Best, and Jean-Michel Ménard.

Department of Physics, University of Ottawa,
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Terahertz time-domain spectroscopy (THz-TDS) is a broadband optical characterization technique widely used for non-invasive imaging and tracing low-energy dynamics in materials. A typical THz-TDS system relies on an ultrashort near-infrared (NIR) pulse focused into second-order nonlinear crystals for the generation and detection of phase-locked THz pulses. Although these systems are undoubtedly beneficial to scientific research and development, the access to a broadband, compact, and affordable THz spectrometer is still a major obstacle to most scientists. Here, we present a portable THz-TDS system employing a cost-effective optical source and components. More importantly, this system incorporates a fiber-based peak field enhancer and a noncollinear geometry to perform broadband and sensitive spectroscopy.

Fabrication and characterization of graphene oxide and reduced graphene oxide thin films

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Department of Physics, University of Ottawa, Ottawa, ON, Canada K1N 6N5

Graphene oxide (GO) and its reduced form have received considerable interest from researchers due to its ease of fabrication and its dispersibility in liquid water. Here, we present the fabrication and characterization of GO and chemically reduced graphene oxide (rGO) thin films deposited onto glass substrates via spray pyrolysis. The rGO is fabricated with two chemical reduction methods based on hydrazine hydrate; the first method uses the reducing agent in vapor phase, producing rGO_V, and the second in liquid phase, producing rGO_L. Exploiting Raman, Fourier-transform infrared, UV-Vis-NIR spectroscopies and I-V measurements, we confirm that the reduction process for rGO_V is susceptible to introducing intercalated water molecules in the material while the fabrication technique for rGO_L is a suitable route to obtain a material with minimal lattice disorder and properties approaching those of graphene.

Terahertz vibrational polaritons

Ahmed Jaber, Avinash Singh, Michael Reitz, Ali Maleki, Yongbao Xin, Brian Sullivan, Robert Boyd, Ksenia Dolgaleva, Claudiu Genes, and Jean-Michel Ménard

Department of Physics, University of Ottawa,
Ottawa, ON, Canada K1N 6N5

When molecular vibrational resonances are coupled to the photonic mode of a cavity, hybridized light-matter states are created. The creation of these polaritonic modes have been shown to modify the properties of the molecules, notably affecting chemical reaction rates and solid-state carrier dynamics. We demonstrate strong coupling between the molecular vibrational resonance of glucose in the terahertz and a planar cavity system.

Sensitive detection of THz photons

Défi Junior Jubgang Fandio, Aswin Vishnu Radhan, Eeswar Yalavarthi, Nicolas Couture, Wei Cui, Angela Gamouras, and Jean-Michel Ménard

Department of Physics, University of Ottawa, Ottawa, ON, Canada K1N 6N5

We investigate the parametric up-conversion and down-conversion of near-infrared photons in a second-order nonlinear crystal as a tool for sensitive detection of terahertz (THz) photons. The parametric conversion process is monitored experimentally as a near-infrared pulse interacts with coherent THz field in 110-oriented GaP crystal. Results show the generation of spectral sidebands consistent with theory. This technique paves the way towards a new generation of THz spectroscopy experiments and quantum experiments relying on few photon detection sensitivity.

STM of Magnetic Topological Insulators

Ryan Plumadore[1], **Leena Aggarwal**[1], **Yanglin Zhu**[2], **Yingdong Guan**[2], **Zhiqiang Mao**[2], **and Adina Luican-Mayer**[1]

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$MnBi_2Te_4$ has been considered the first intrinsic antiferromagnetic topological insulator, where tremendous research has been done both theoretically and experimentally. But the complete understanding of its theoretical prediction for anomalous hall and axionic phases is still contested experimentally. Here, in this work, we observe the electronic gapless surface states in MnBi2Te4 using low-temperature (~10K) scanning tunneling microscopy/spectroscopy (STM/STS). We observe that the surface states are spatially inhomogeneous which might be due to non uniform magnetic ordering, induced by surface defects or magnetic spin fluctuations. The direct observation of gapped spectroscopy at few surfaces due to breaking of time reversal symmetry is suggestive of the presence of strong magnetic field of $MnBi_2Te_4$. Additionally, the appearance of localized edge states at odd-even edges of $MnBi_2Te_4$ indicate both QAH and axion states in the system.

Broken Sublattice Symmetry Effects and Phase Transitions in Triangular Artificial Graphene Quantum Dots

Yasser Saleem[1], **Amintor Dusko**[1], **Moritz Cygorek**[1], **Marek Korkusinski**[2], **and Pawel Hawrylak**[1]

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We describe here the effects of broken sublattice symmetry, and the emergence of a phase transition in triangular artificial graphene quantum dots with zigzag edges[1]. The system consists of a structured lateral gate confining two dimensional electrons in a quantum well into artificial minima arranged in a hexagonal lattice. The sublattice symmetry breaking is generated by forming an artificial triangular graphene quantum dot with zigzag edges. The resulting Hamiltonian generates a tunable ratio of tunneling to strength of electron-electron interactions and a degree of sublattice symmetry with control over shape. Using a combination of tight binding, Hartree-Fock and configurations interaction methods we show that the ground state transitions from a metallic to an antiferromagnetic insulating phase by changing the distance between sites or depth of the confining potential. At the single particle level these triangular dots contain a macroscopically degenerate shell at the Fermi level. The shell persists at the mean-field, Hartree Fock level for weak interactions in the metallic phase but disappears for strong interactions and antiferromagnetic insulating phase. We determine the effects of electron-electron interactions on the ground state, the total spin, and the excitation spectrum as a function of filling of the system away from half-filling. We find that the half-filled charge neutral system leads to a fully spin polarized state in both metallic and antiferromagnetic regimes in accordance with Lieb's theorem. In both regimes a relatively large gap separates the spin polarized ground state to the first excited many-body state at half-filling of the degenerate shell, but by adding or removing an electron, this gap drops dramatically, and alternate total spin states emerges with energies nearly degenerate to a spin polarized ground state.

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Kitaev chains and rings: Majorana Zero Modes and artificial gauge

David J. Gayowsky, Amintor Dusko, Jacob Manalo, Mahan Mohseni, and Pawel Hawrylak

Department of Physics, University of Ottawa, Ottawa, Canada

We present here a theory of electronic properties of chains of quantum dots on p-type superconductors, proposed originally by A. Y. Kitaev as a means to realise Majorana Zero Modes. A fluctuating number of electrons tunnel from dot to dot and form Cooper pairs on neighboring dots. We use exact diagonalisation to determine ground and excited states of Fermions on a chain. In parallel, we define Majorana Fermions on each dot, and bond Fermions built from Majorana operators on neighboring dots. We diagonalise the Hamiltonian in bond Fermions, and find the nonlocal bond fermion built from Majorana operators at the beginning and end of a chain missing from the Hamiltonian. For it to appear to match the energy spectrum obtained by exact diagonalisation it must be added with zero energy. We next introduce coupling between the first and last dot, and study the evolution of the electronic properties from chain to ring. On a ring we discuss an artificial gauge which affects the motion of Cooper pairs. Finally, we discuss the effect of the artificial gauge on nonlocal bond fermions.

Reinforcement learning configuration interaction

L. Szulakowska, Roman Krems

Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, Canada

Designing quantum devices requires vast theoretical exploration of strongly correlated systems by solving Schrodinger's equation in the space of all possible Slater determinants (SD) [1]. In practice, full configuration interaction (FCI), is often too costly for strongly correlated systems, i.e. if a single SD approximation is insufficient. Methods with iterative growth of the SD space exist, but they require many diagonalization instances in a growing selected space. Machine learning offers promising alternative strategy by learning the relation between a SD subspace and the ground state (GS), which can be exploited without increasing the computational resources [1-3].

In this work, we consider a reinforcement learning approach [4-5], which involves an agent gradually learning the best course of action in a given observed state. It is trained by exploring the environment, performing different actions and receiving reward signals. This method requires very little memory to store the experiences and in principle needs no label generation or prior knowledge of the system, which are obstacles in other supervised learning methods.

We use the double deep Q-learning with dueling architecture [6-7]. The observations (observed states of the environment) are defined as linear combinations of n SDs of N electrons up (and N electrons down, with Sz=0) on M single particle energy levels. The agent's reward is the difference in energy ΔE between the GS of two observations. The action of moving between observations involves addition of a single SD, while another one is removed at the same time. We propose a form of universal action transferable across problems with variable n, N and M. This opens the possibility of extrapolation applications, with experience gained from smaller problems used for solving larger ones [8].

We first consider the simplest example of N=2, M=12, for interacting electrons within a parabolic MoS_2 quantum dot. The action is encoded as a pair of occupied energy level indices, which define a N=2 configuration to be added to the current observation. Training is performed in episodes, as agent transitions from one observation to another. We design a curriculum of episodes of gradually increasing difficulty – the larger the ΔE, the simpler the episode. We show that the agent improves at harder tests while the reward grows and GS energy decreases. This approach promises considerable calculation speedup for any correlated problem, as an alternative to FCI, or in place of the initial guess for iterative methods [2].

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Electronic properties and transport in WTe_2 monolayer topological insulators with strong disorder

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In the following work we report our theoretical investigation of 1-T' WTe_2 monolayer Z2 topological insulator nanoribbons in the presence of the strong Anderson-type disorder. We focus on the comparison of two types of edge orientations. First, we discuss how scanning tunneling microscopy can distinguish between two types of edge in relation to a vastly different position of the 1D Dirac cone with respect to bulk band edges. In next step we show that transport via quantum spin Hall edge states is robust for heavily disordered samples due to their anomalously small localization length. However, for the same disorder strength, the resistance measurement for perpendicular set of gates can qualitatively differ, allowing for further identification of the type of edge. We find that when temperature effects are included, conductance G(T) is also sensitive to both disorder strength, responsible for localization of bulk states, as well as edge termination. We also make the case that an increase in resistance from short to long channel transport in WTe_2 devices is consistent with a heavily disordered system related to Anderson transition in the topological system. We conclude with study of the Luttinger parameter K in this system.

Synthetic correlated electron system with twisted bilayer graphene quantum dots

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Synthetic correlated electron systems offer the possibility to design topological quantum matter with properties vastly different from its constituents, with superconductivity, ferromagnetism and incompressible liquids of the fractional quantum Hall effect as good examples. Electronic correlations and entanglement associated with it, originate from electron-electron (e-e) interactions in a flat band (i.e. degenerate electronic shells). Recently, two systems, allowing design of the degenerate electronic shells, were proposed: triangular graphene quantum dots with zigzag edges (TGQD)[1-3] and magic angle twisted bilayer graphene (MATBG) [4].

In this work, we combine the two approaches to build a synthetic correlated electron system by combining two triangular graphene quantum dots with zigzag edges into a bilayer TGQD [3]. We study the effect of the moiré potential on the internal structure and wave function properties of the zero-energy shell. We also investigate the possibilities of manipulating moiré/field-confined QD-like states properties, e.g. state symmetry, using the twist angle as a new mean of control.

We use an ab initio fitted tight-binding model with tunnelling matrix elements covering up to the 6th nearest neighbours [5] and study the formation of the moiré patterns and creation of the flat bands in graphene quantum dots consisting of up to one million atoms as a function of misaligned angles.

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Fine structure of excitons in TMD type-II heterostructures

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We describe here the electronic and optical properties of $MoSe_2/WSe_2$ type-II heterostructure using ab initio methods and tight-binding (TB) approximation coupled with solution of Bethe-Salpeter equation (BSE) yielding excitonic spectrum [1]. We start with determining the electronic structure of MoSe2/WSe2 from first principles. We obtain type-II band alignment and conduction band minima at Q points. Then we perform analysis of Kohn-Sham wavefunctions allowing to detect leading layer and spin contributions. Next, we construct minimal TB model for $MoSe_2/WSe_2$ heterostructure, which allow us to understand orbital contributions to Bloch states and study the effect of wavefunctions on the excitonic spectrum. We accurately solve BSE and determine the exciton fine structure due to type-II spin-split band arrangement [2] and topological moments, considering both A/B, spin bright/dark and intra-/interlayer exciton series using simplified Rytova-Keldysh non-local screening theory. In next step we analyse effect of moiré potential and compare it with fully tight-binding approach to excitons in twisted heterostructures.

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Spin-valley qubits in gated quantum dots in a single layer of transition metal dichalcogenides

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We describe operation of spin-valley qubits in gated quantum dots in a single layer of transition metal dichalcogenites (TMDCS) [1]. The spin valley qubit is described by a microscopic tight-binding [1,2,3] model suitable for accurate description of multi-million atom nanostructures compatible with existing experiments [4,5]. We obtain two degenerate qubit states, belonging to the two non-equivalent valleys, each with the opposite-spin, built by conduction band states of even parity with respect to the metal plane. We rotate the qubit by logical σx operation which requires simultaneous transition between opposite spin states in each valley and between the two nonequivalent valleys. We show that a time dependent perpendicular electric field coupling even and odd orbitals, spin orbit interaction and highly localized lateral potential are needed to rotate the qubit enabling transition to the opposite valley and spin qubit state.

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Single-dopant band bending fluctuations in $MoSe_2$ measured with electrostatic force microscopy.

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In this work, we measured the bias-dependent surface potential of exfoliated multilayer $MoSe_2$ on SiO_2 with frequency-modulated atomic force microscopy. We also modelled this system as a 1D metal-insulator-semiconductor (MIS) capacitor. Bias-dependent two-state fluctuations in the capacitor force were measured. This two-state effect arises due to a change in global band bending as an electron moves into and out of an acceptor state. It is not due to a varying Coulomb potential of an electrically isolated state being occupied and unoccupied. Importantly, the amplitude of this random telegraph noise can be fully explained as being due to the bias-dependent surface potential, and does not depend specifically on the energy levels of the acceptor states themselves. Finally, we demonstrate a methodology that may be used to provide an order-of-magnitude estimate of band bending (i.e. charge reorganization) timescales for an energetically conservative system. These timescales, which in this work are on the order of 30 ns, exhibit strong bias and spatial dependence.

Edge states and strain driven topological phase transitions in HgTe topological insulator square quantum dots

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We present here a theory of the electronic properties of quasi two-dimensional HgTe square quantum dots made of a topological insulator. The topological insulator is described by a four-band Bernevig-Hughes-Zhang (BHZ) Hamiltonian. The trivial versus topological properties of the BHZ Hamiltonian were characterized by the different topologies that arise when mapping the in-plane wavevectors through the BHZ Hamiltonian onto a Bloch sphere. In the topological insulator square quantum dot, edge states were formed with quantum barriers in the corners. We explicitly related the emergence of edge states to the transition from the trivial to the nontrivial topological regime by straining the topological insulator square quantum dot.

Reversible local response of domain wall networks in ferroelectric interfaces of marginally twisted WS_2 bilayers

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Semiconducting ferroelectric materials with low energy polarisation switching offer a platform for next-generation electronics such as ferroelectric field-effect transistors. Ferroelectric domains at symmetry-broken interfaces of transition metal dichalcogenide films provide an opportunity to combine the potential of semiconducting ferroelectrics with the adaptability of two-dimensional material devices. Here, local control of ferroelectric domains in a marginally twisted WS_2 bilayer is demonstrated with a scanning tunneling microscope, and their observed reversible evolution understood using a string-like model of the domain wall network. We identify two characteristic regimes of domain evolution: (i) elastic bending of partial screw dislocations separating smaller domains with twin stacking and (ii) formation of perfect screw dislocations by merging pairs of primary domain walls. We also show that the latter act as the seeds for the reversible restoration of the inverted polarisation.

Towards quantum computer based on topologically protected qubits

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We describe the potential realization of a synthetic Haldane spin-1 chain in an array of InAsP quantum dots embedded in an InP nanowire for the possible construction of a topologically protected singlet-triplet qubit. The quantum dots are defined by a random distribution of arsenic atoms. Using an ab-initio derived tight-binding Hamiltonian for a single and a double InAsP quantum dot containing millions of atoms, the single particle states were obtained. Despite the random distribution of As atoms, the conduction band states of a single dot could be understood in terms of macroscopic s, p, and d quantum dot orbitals and a tunneling between the dots for the double dot system. Next, we filled the quantum dot orbitals with N-electrons. The many-body Hamiltonian in the basis of N-electron configurations, including Coulomb interactions was then constructed with the single particle states from the tight-binding model. Using exact diagonalization, we have determined that for a single quantum dot with a filled s-shell and half filled p¬-shell, the ground state has a total electronic spin of S = 1 and that the ground state for a double dot system is a singlet state with a total spin of S = 0, which is consistent with Heisenberg model [1]. The low-energy spectrum of the double quantum dot array was then successfully fitted to both the Hubbard-Kanamori and Heisenberg model Hamiltonians to confirm that the quantum dot array with 4 electrons in each dot hosts the Haldane quasipartcles of a spin-1 chain. We then used the density matrix renormalization group (DMRG) method [2] to obtain the low energy spectra of a 50 quantum dot chain using the Hubbard-Kanamori model and determined that the singlet and triplet states approach degeneracy and are separated by an energy gap from the quintuplet state as is the case with the Heisenberg spin-1 model.

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