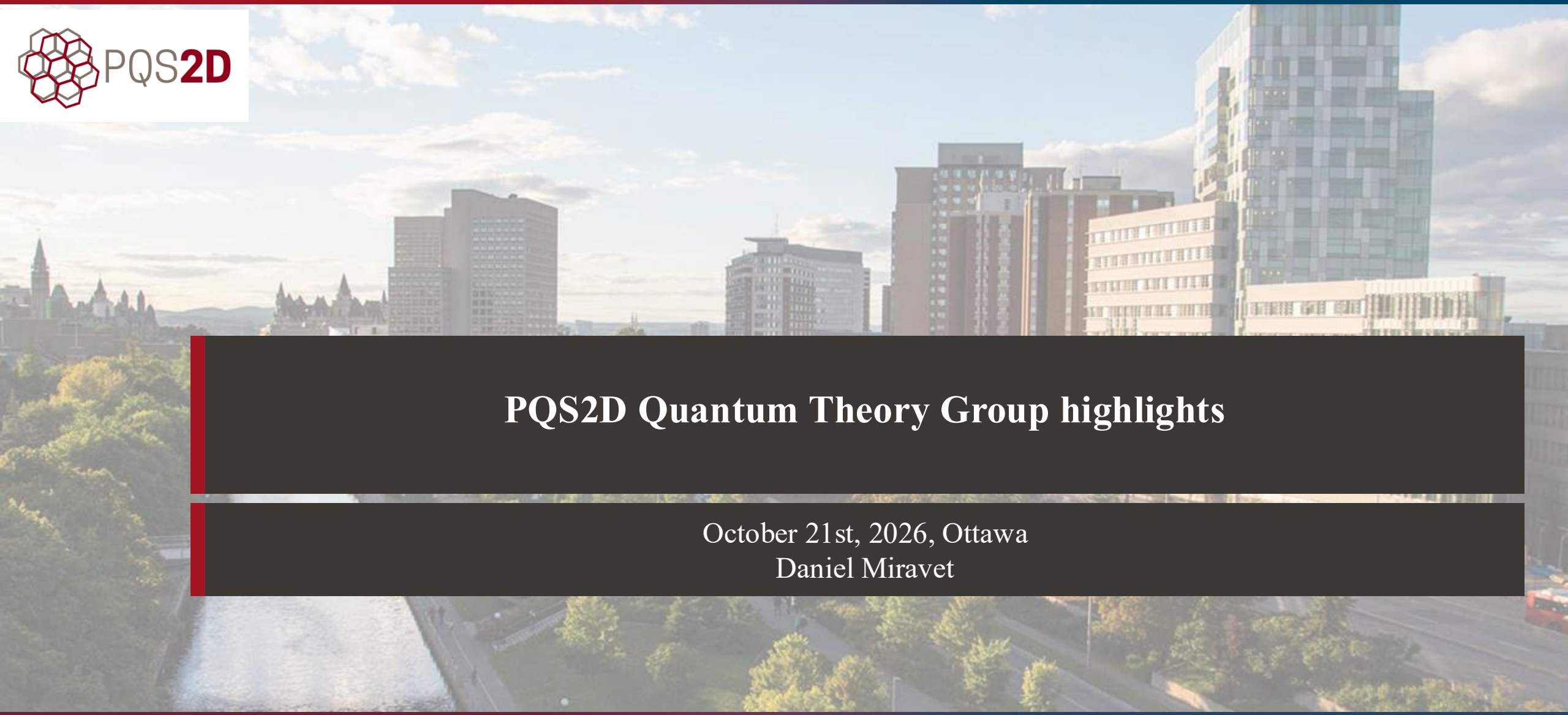


PQS2D Quantum Theory Group highlights

October 21st, 2026, Ottawa

Daniel Miravet

Thrusts and this year's output

Thrust 1
Moiré heterostructures

PUBLISHED

- Twisted trilayer graphene: magnetism and hidden quantum geometry
  Sci. Rep. 2026

IN PROGRESS

- Atomistic simulation of quasicrystals
  with Luican-Mayer group
- Billion-atom Hartree-Fock with MPS and tensor cross interpolation
- Moiré excitons

Thrust 2
Gated quantum dots as simulators

PUBLISHED

- Excitonic complexes in gated WSe_2 QDs
  PRB 110, 2024
- Optics of BLG QDs with trigonal warping
  PRB 110, 2024
- BLG QD chains simulate the Haldane phase
  PRL 136, 2026
- Two-qubit gate with Haldane singlet-triplet qubits
  PRB 111, 2025
- Majorana modes in QD chains with VQE
  pss(b) 262, 2025

IN PROGRESS

- Artificial moiré lattices from QD arrays on a 2D material
  with Gaudreau group
- Landau levels and many-body interactions in WSe_2
  with Gaudreau group
- Nitrogen impurities in graphene QDs

Thrust 3
Large-area 2D materials

IN PROGRESS

- GW-BSE code set up
- Optical properties of MOCVD-grown materials

Thrust 1: Moiré Heterostructures as Quantum Simulators

Twisted trilayer graphene turns antiferromagnetic at weaker U than other multilayers

scientific reports

OPEN

Magnetism and hidden quantum geometry in charge neutral twisted trilayer graphene

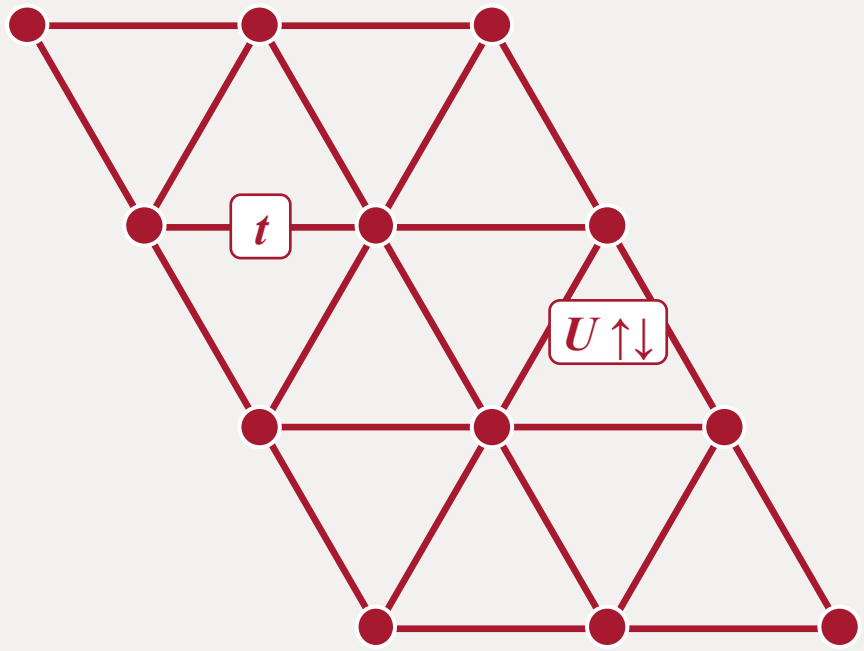
Alina Wania Rodrigues[1]✉, Maciej Bieniek[2], Daniel Miravet[1] & Paweł Hawrylak[1]

- Mirror-symmetric TTG in the **mean-field** approximation, with **electric field** and **hBN strength** as tuning parameters

Co-authors: A. Wania Rodrigues, M. Bieniek, D. Miravet

Moiré Hubbard simulator:

$$H = -t \sum_{<i,j>} c_i^{\dagger} c_j + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



Thrust 1: Moiré Heterostructures as Quantum Simulators

Atomistic LDOS maps of relaxed moiré lattices

Joint work with the Luican-Mayer group; Sean Walker reports the experiment

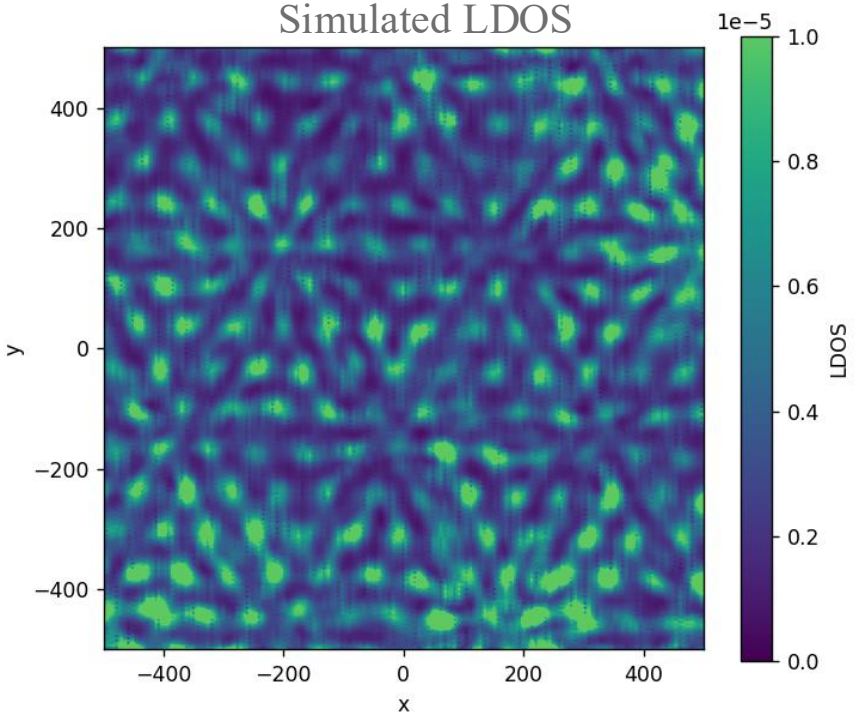
Lattice relaxation → **Tight-binding spectrum** → **Topology and e-e interactions**

↓

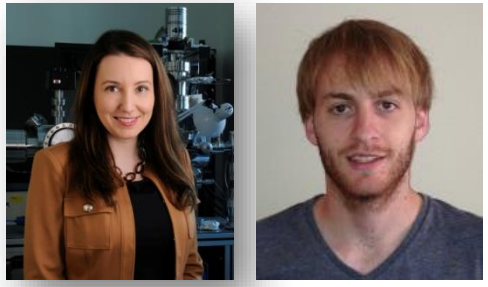
Scaling up: MPS + tensor cross interpolation
Hartree-Fock for billion-atom moiré samples

Work in progress
Moiré excitons

Simulated LDOS



Experimental collaborators:



Co-authors: A. Wania Rodrigues, M. Bieniek, M. Korkusiński, D. Miravet

Thrust 2: Gated Quantum Dots as Simulators

Atomistic theory of gated dots predicts exciton binding, optical spectra and artificial lattices

PRB 110, 235404 (2024)

Excitonic complexes in gated WSe_2 QDs

- Gate confines holes but **repels electrons** (type-II)
- Tests whether e-h attraction overcomes gate repulsion; gives absorption spectrum

PRB 110, 155421 (2024)

BLG QDs with trigonal warping

- Shallow dots are dominated by **three minivalleys** around each K
- Bethe-Salpeter excitonic spectrum

In progress

Landau levels and many body interactions in WSe_2

- Interplay of LL physics with Coulomb interactions

In progress

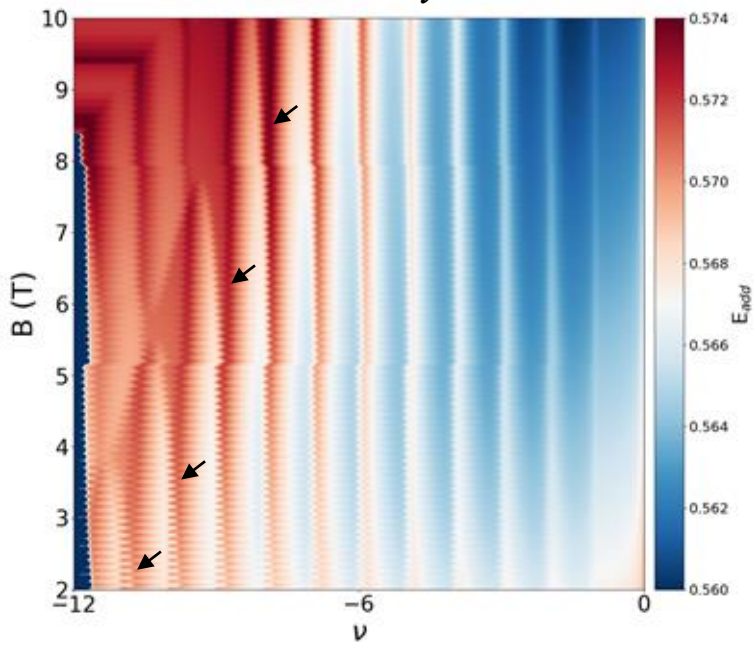
Artificial moiré lattices from QD arrays

- A periodic array of gated QDs imposes an artificial moiré potential on a 2D material
- Lattice geometry and depth set by the gates rather than by twist angle

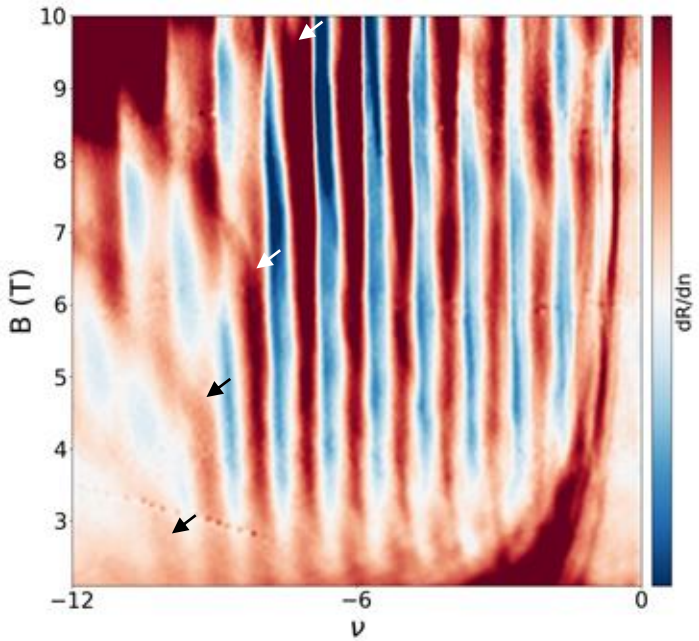
Co-authors: D. Miravet, M. Albert, A. Wania Rodrigues, M. Korkusiński

Thrust 2: Strong Interactions and Spin-Orbit Coupling in 2D Systems

Theory

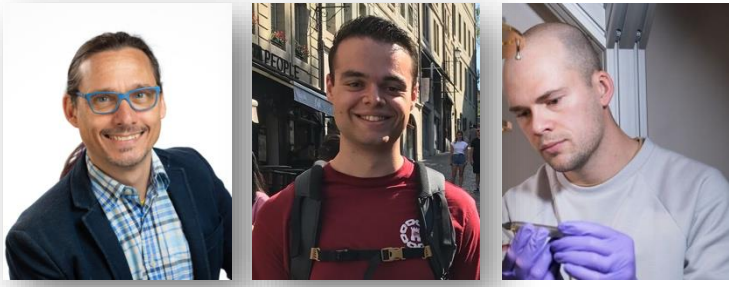


Experiment



- Theoretical model: **massive Dirac fermion** in a magnetic field
- Discontinuities in the addition spectra – signatures of **strong interactions**
- Study of possible GS configurations reveals **multi-hole depolarization** events

Experimental collaborators:



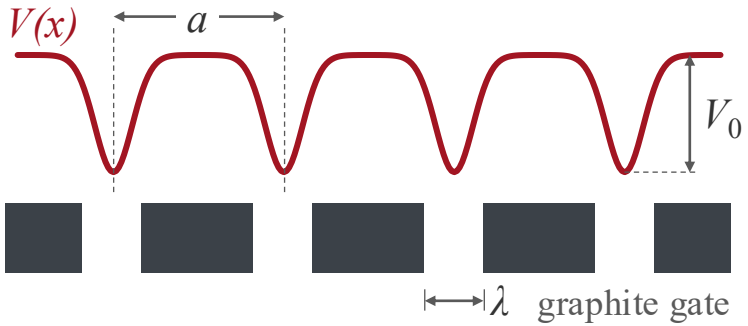
Co-authors: A. Wania Rodrigues, M. Korkusiński

Thrust 2: Designing Artificial Moiré

A patterned graphite gate imposes a tunable moiré potential on monolayer WSe_2

Gate potential

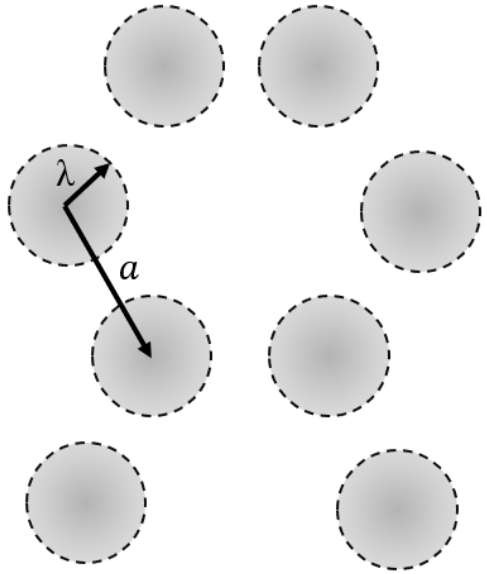
Side view: each hole in the graphite gate creates a **Gaussian well**



- **Pitch** a: lattice spacing
- **Width** λ: well size
- **Depth** V_0: set by the gate voltage

Model

Hexagonal patterned-hole lattice



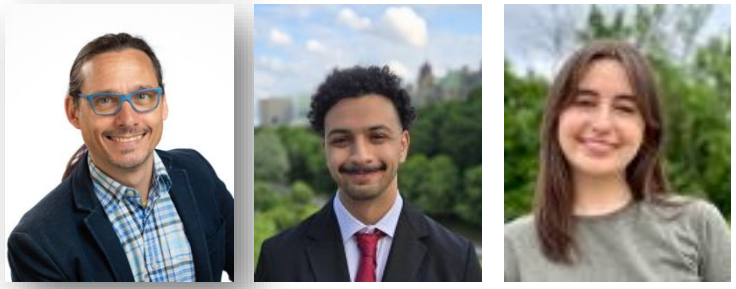
Hole pattern → periodic **Gaussian potential**

Tuning and team

Two knobs set the moiré depth:

- **Theory:** Gaussian depth, inter dot distances, etc.
- **Experiment:** applied electric field

Experimental collaborators:



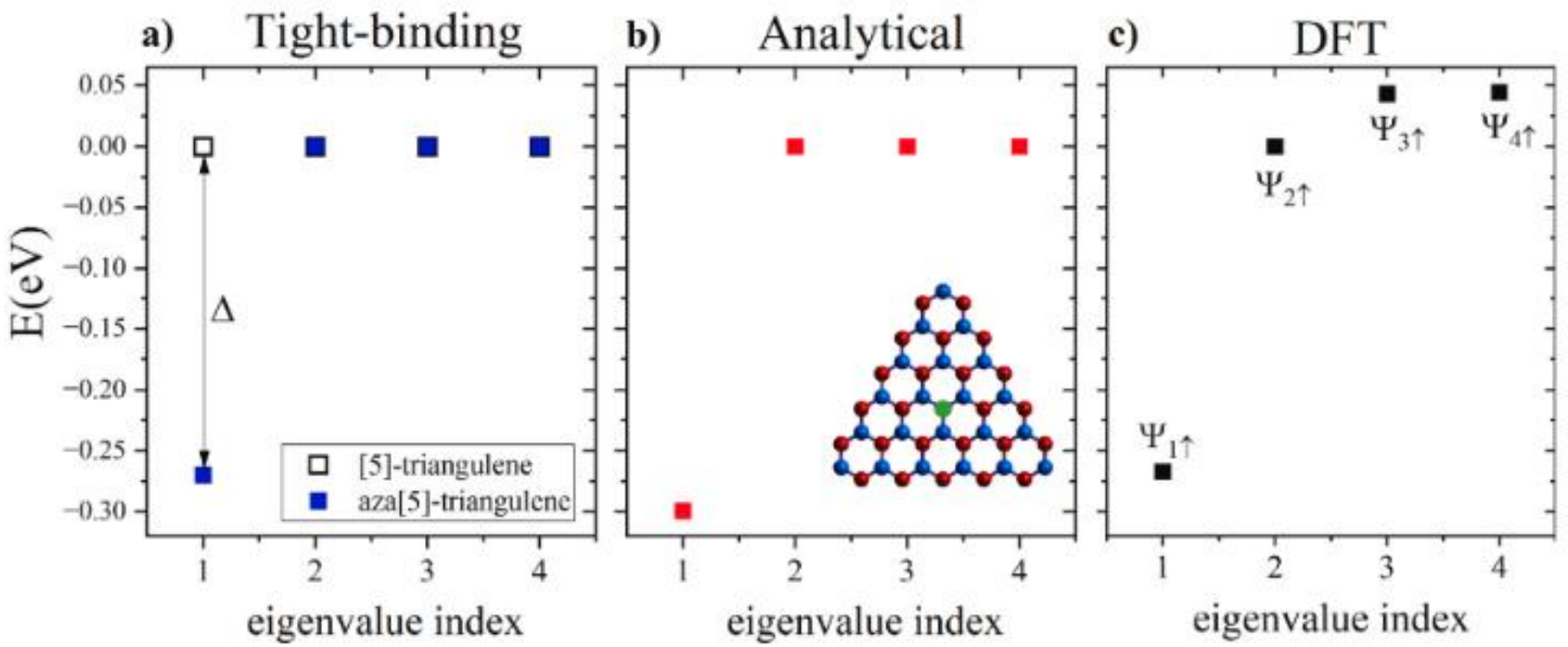
Co-authors: A. Wania Rodrigues, M. Korkusiński

Thrust 2: Impurities in Graphene QDs

Atomistic theory of graphene quantum dots now includes nitrogen impurities

Thrust 2
Impurities in graphene QDs

- Theory of **graphene quantum dots with nitrogen impurities**
- **DFT + configuration interaction** for N impurities on graphene



Co-authors: A. Wania Rodrigues, S. Abedi, M. Islam, D. Miravet

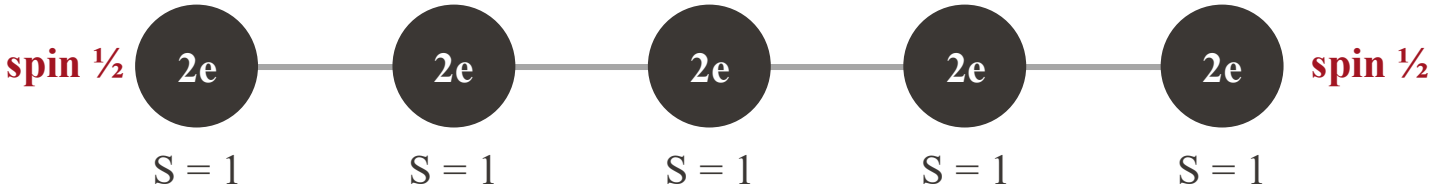
Thrust 2: BLG Dots Simulate Haldane Matter

A chain of bilayer graphene dots with two electrons each simulates the Haldane spin-1 chain

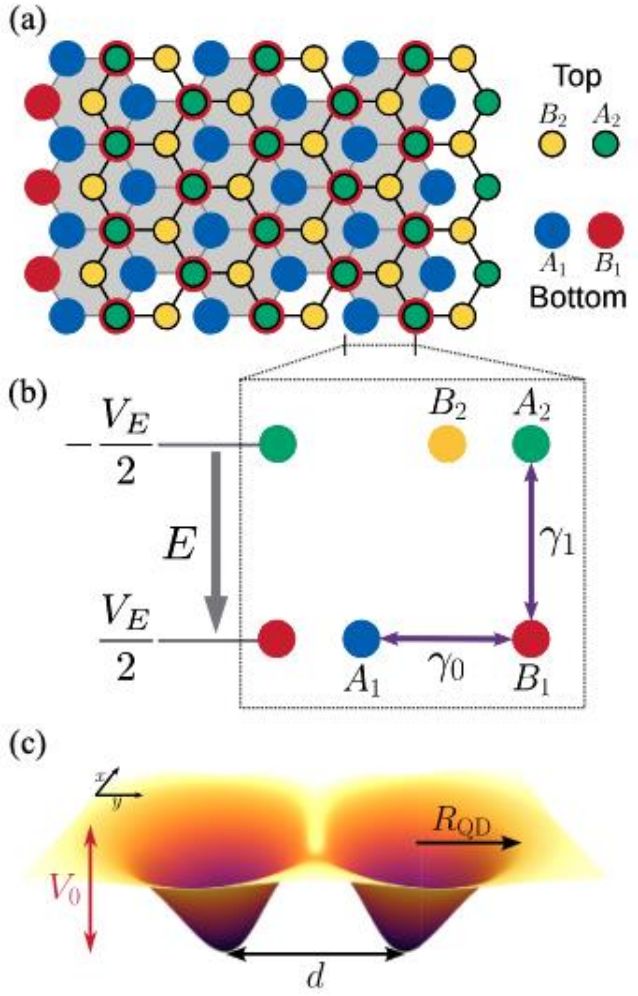
PHYSICAL REVIEW LETTERS **136,** 086604 (2026)

Bilayer Graphene Quantum Dots as a Quantum Simulator of Haldane Topological Quantum Matter

Daniel Miravet,[1,*] Hassan Allami,[1] Marek Korkusiński,[1,2] and Paweł Hawrylak[1]
[1]*Department of Physics, University of Ottawa, Ottawa, Ontario, K1N 6N5, Canada*
[2]*Quantum and Nanotechnologies Research Centre, National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada*



- Two electrons per gated BLG dot form a **spin-1 ground state**
- Coulomb interactions and valley mixing in **one atomistic framework**
- Coupled dots realize the **Haldane phase**, with a free spin ½ at each end of the chain



Thrust 2: BLG Dots Simulate Haldane Matter

Atomistic theory maps the dot chain onto a spin-1 bilinear-biquadratic model

1 **Single dot: atomistic tight binding + exact diagonalization**

Spin and valley polarization transitions vs interaction strength and gates; **spin-1 ground state for N = 2**

2 **Double dot with four electrons**

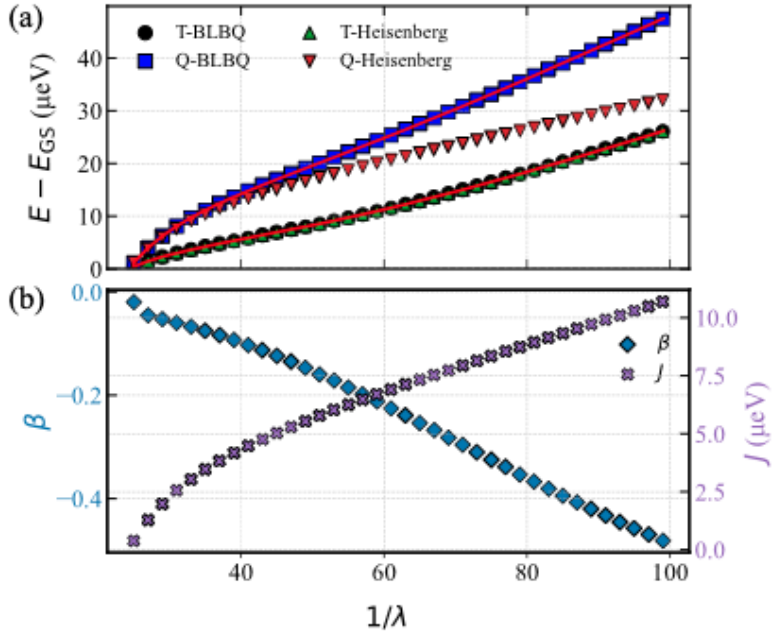
Low-energy spectrum of two coupled dots fixes the spin couplings

3 **Mapping to a spin-1 BLBQ model**

$$H = J \sum_i [S_i \cdot S_{i+1} + \beta (S_i \cdot S_{i+1})^2]$$

4 **Dot arrays simulated with tensor network states**

Haldane phase in a range of gate and interaction parameters



D. Miravet, H. Allami, M. Korkusiński, P. Hawrylak, Phys. Rev. Lett. 136, 086604 (2026)

Thrust 3: Large-Area 2D Materials

First-principles tools for optics of large-area 2D materials are in place

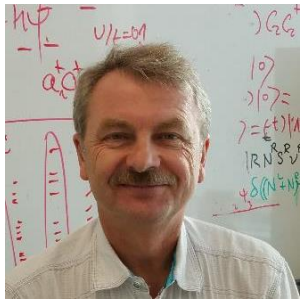
Thrust 3

MOCVD-grown 2D materials

- **GW-BSE code set up** for the calculation of **optical properties**
- Targets materials grown by MOCVD (see H. Chi's talk)

Co-authors: G. Sesti, D. Miravet

Theory Team



P. Hawrylak



M. Korkusiński



A. Wania Rodrigues



M. Bieniek



J. Pawłowski



D. Miravet



H. Allami



M. Islam



M. Albert



S. Abedi



G. Sesti

PQS2D

Thank you!

NSERC CRSNG