Implementation of the bilayer Hubbard model in a moiré heterostructure

Subhradeep Misra

Fakultät für Physik, Munich Quantum Center, and Center for NanoScience, Ludwig-Maximilians-Universität München, München, Germany

Motivation

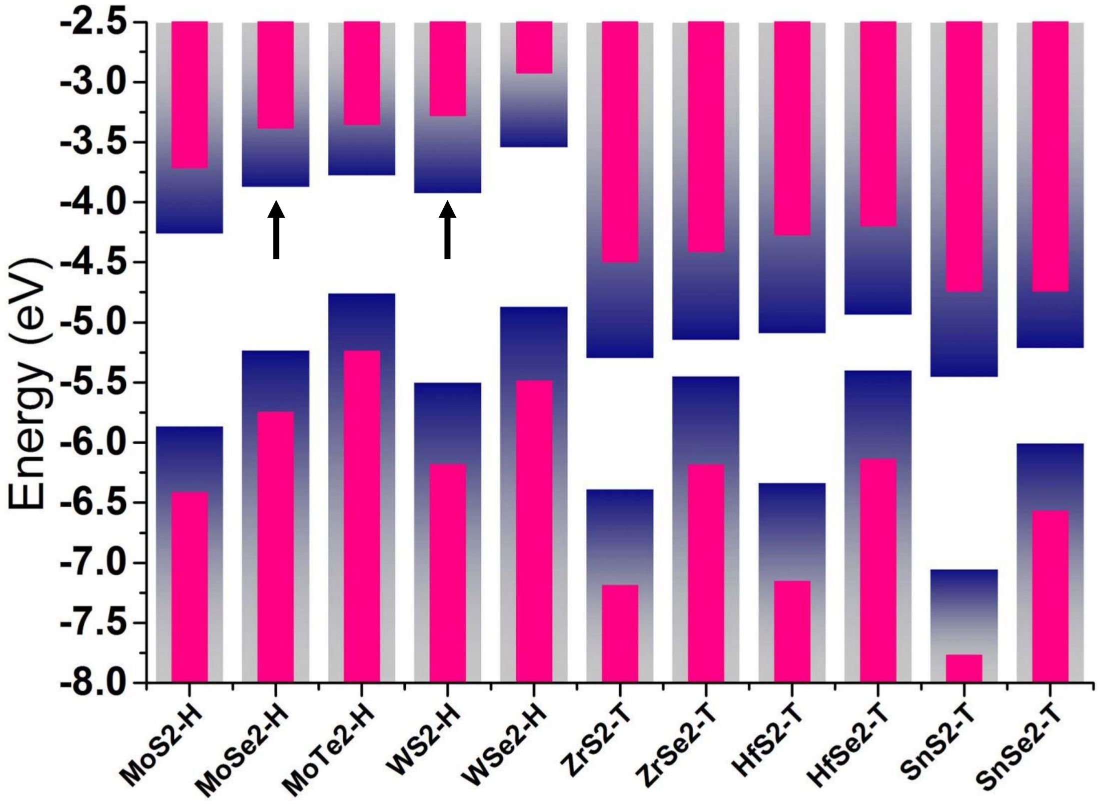
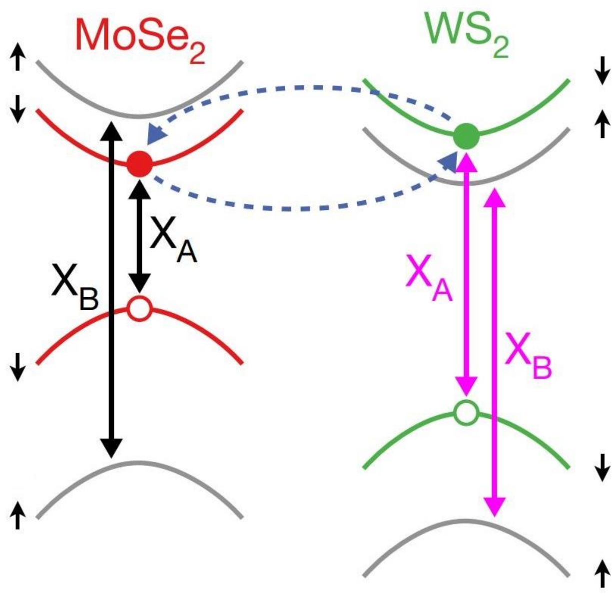


Figure: Position of band edges for stable semiconducting TMDs with respect to vacuum. The band edge of DFT-PBE data and G_0W_0 data are indicated by filled navy blue gradient column and pink solid column, respectively.

Zhang et al., 2D Mater. 4, 015026 (2016)

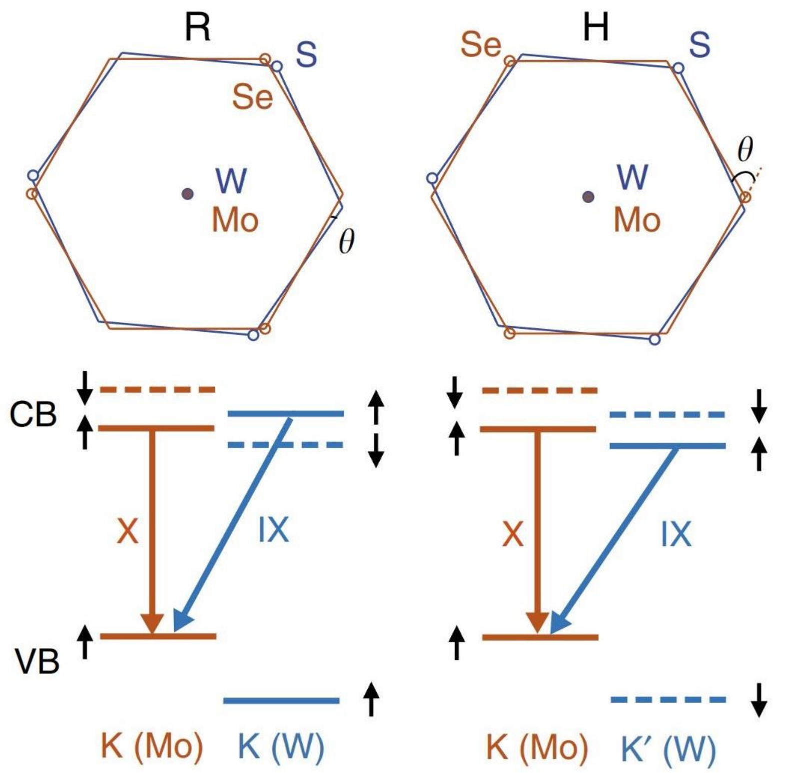
- Calculations reveal near-resonant CBs, facilitating exciton hybridization
- For small twist angles, $MoSe_2/WS_2$ host moiré excitons unveiling correlated physics
- Precise band alignment is still an *open question*!

Experimental insights



*Alexeev, E.M. et al. Nature **567,** 81–86 (2019)*

Type II



*L. Zhang. et al. Nat. Comm. 11**:5888** (2020)*

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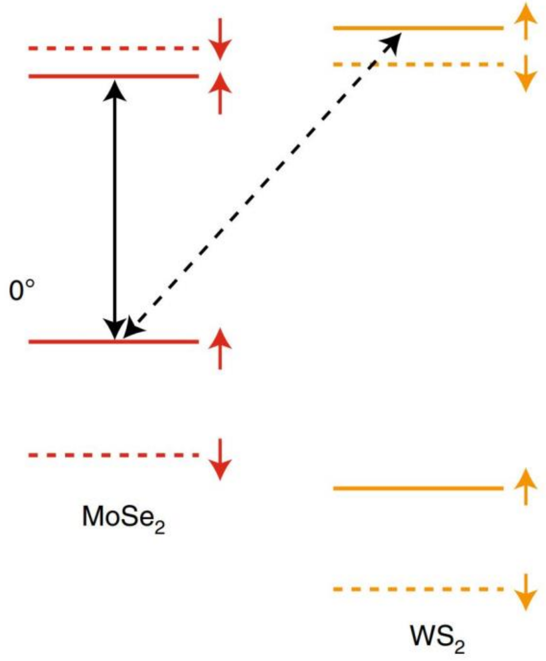
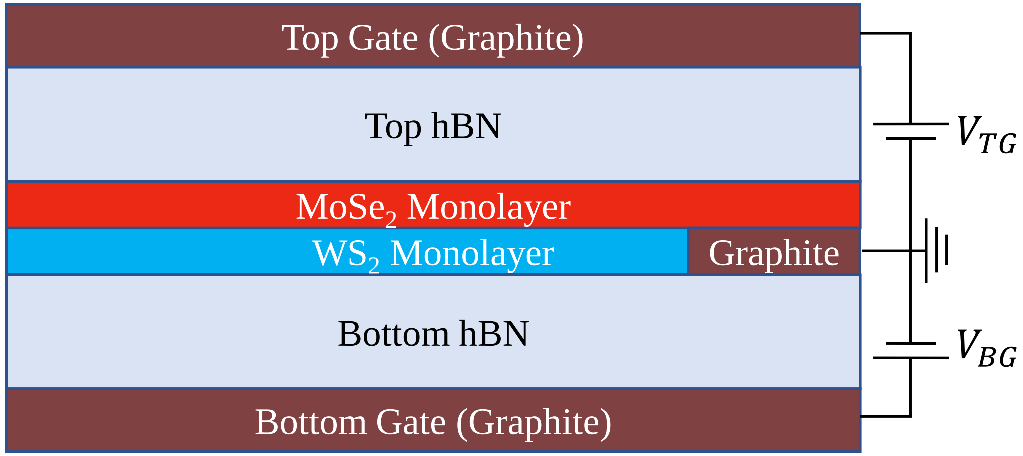


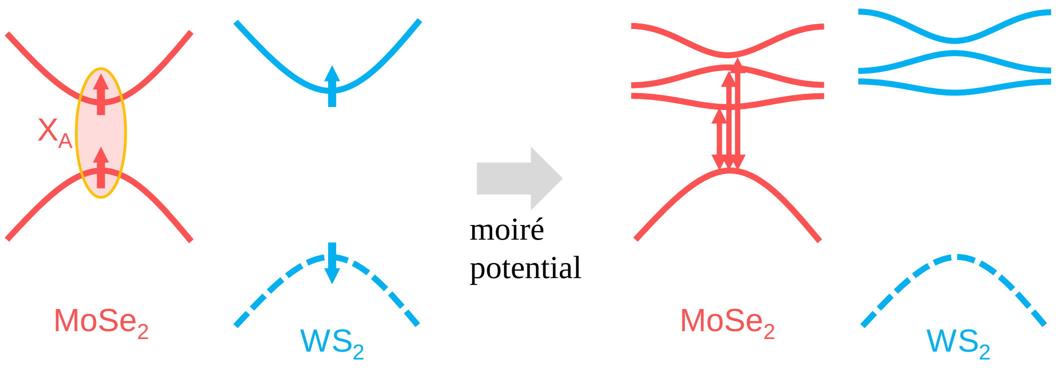
*Tang et al. Nat. Nanotechnol. 16**,** 52 (2021)*

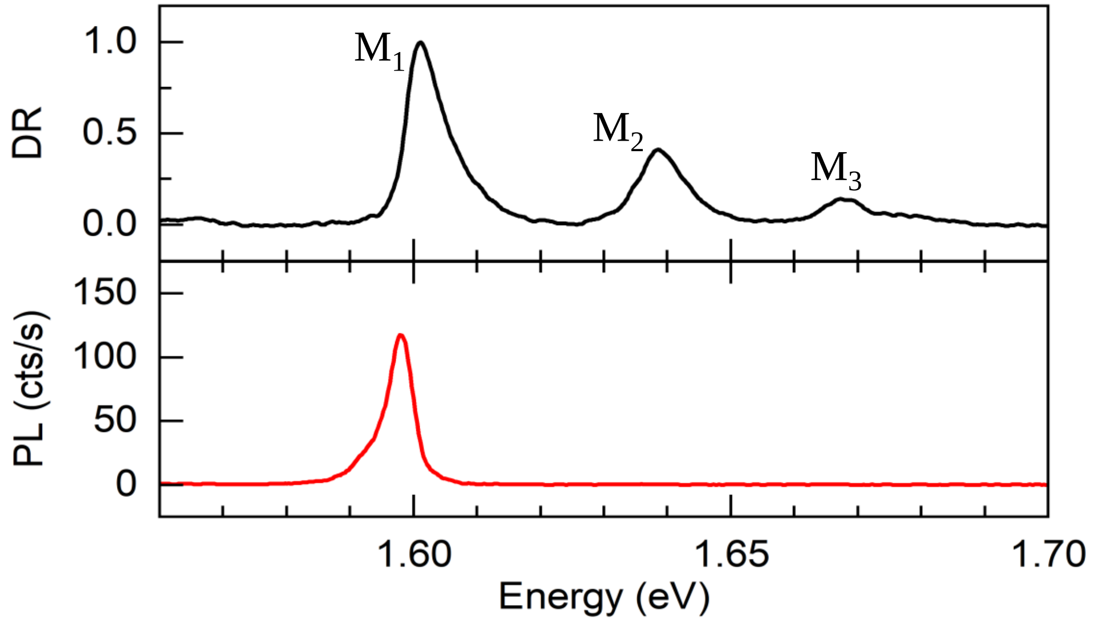
Type I

Moiré excitons in 2H-stacked $MoSe_2/WS_2$



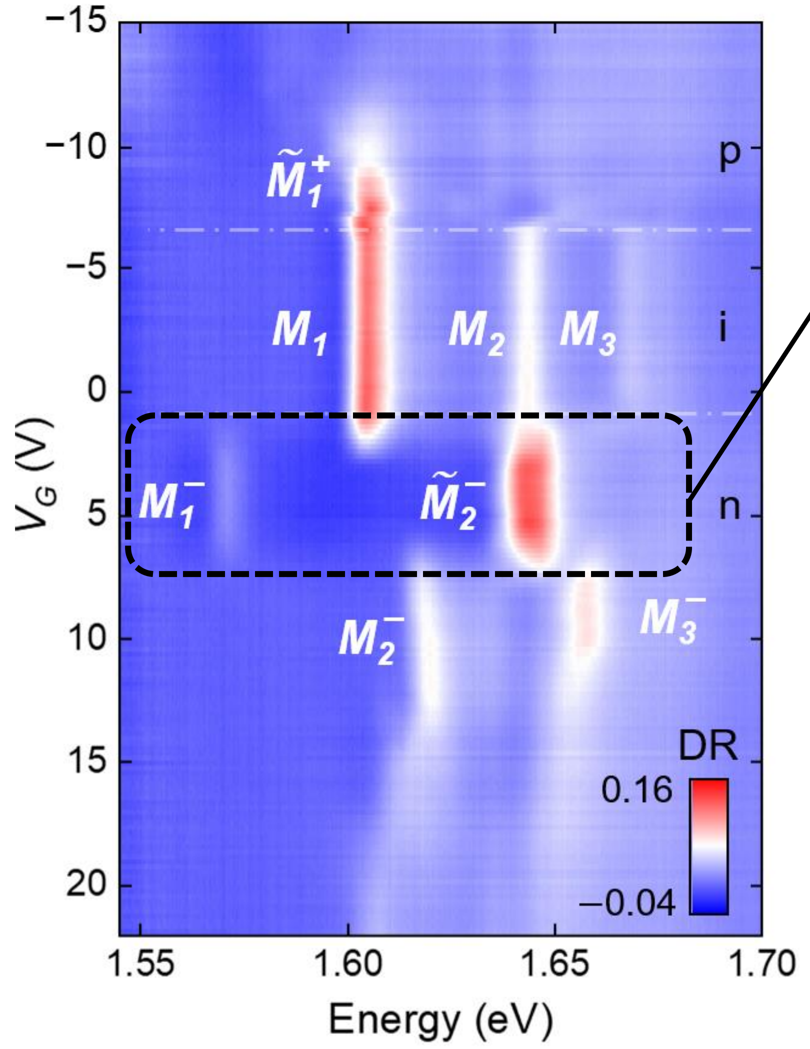
Antiparallelly (60^0, 2H) stacked dual-gated field-effect device



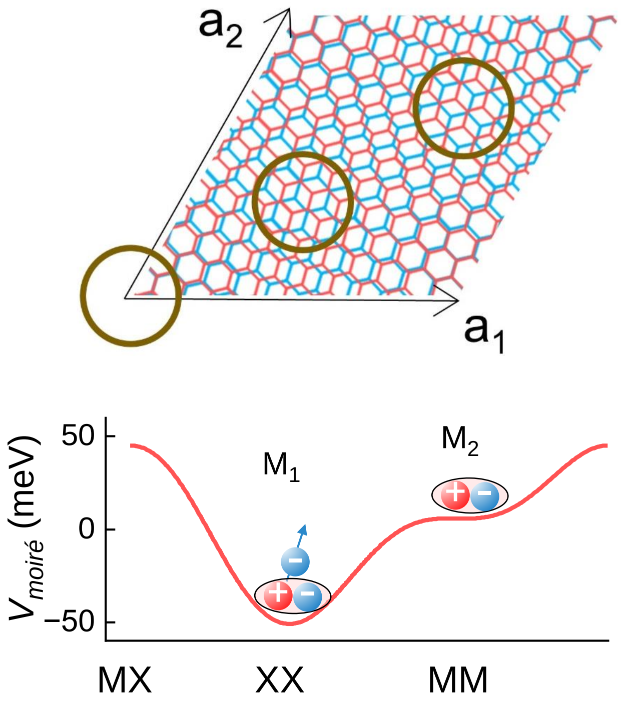


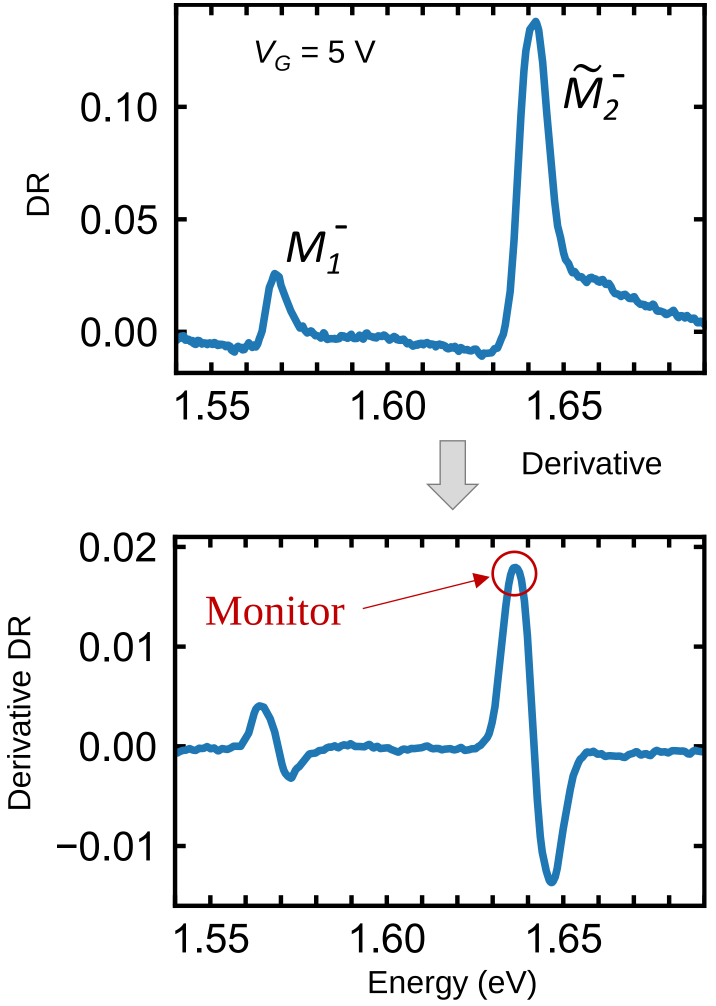
Phys. Rev. Lett. **132**, 076902

Charge doping effects on moiré excitons

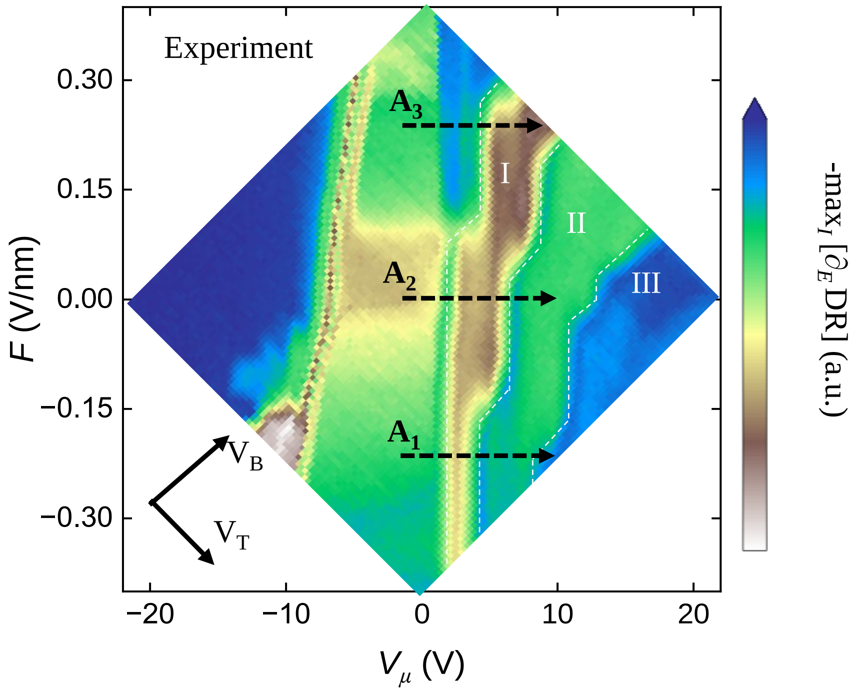


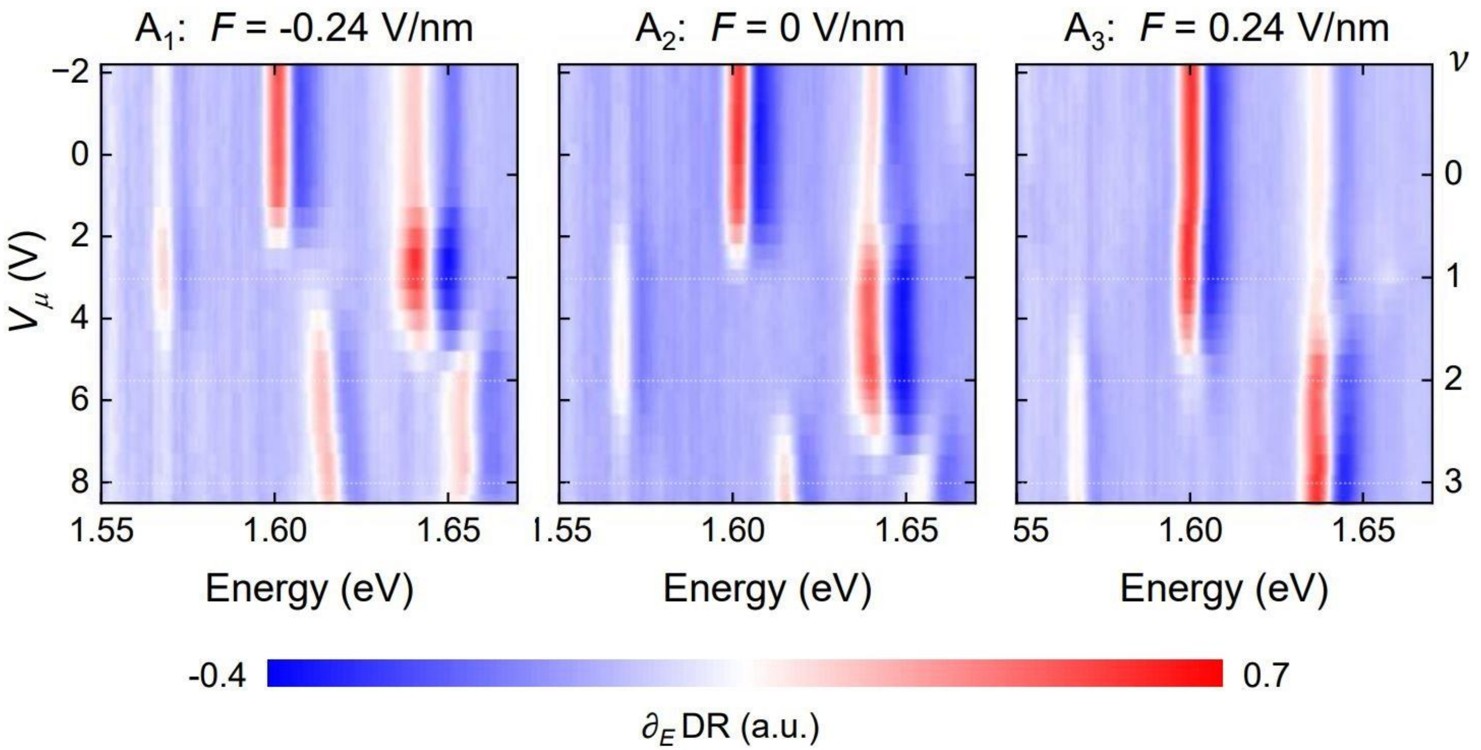
Charged exciton resonances reminiscent of trions





Layer-by-layer charging: electrostatic model





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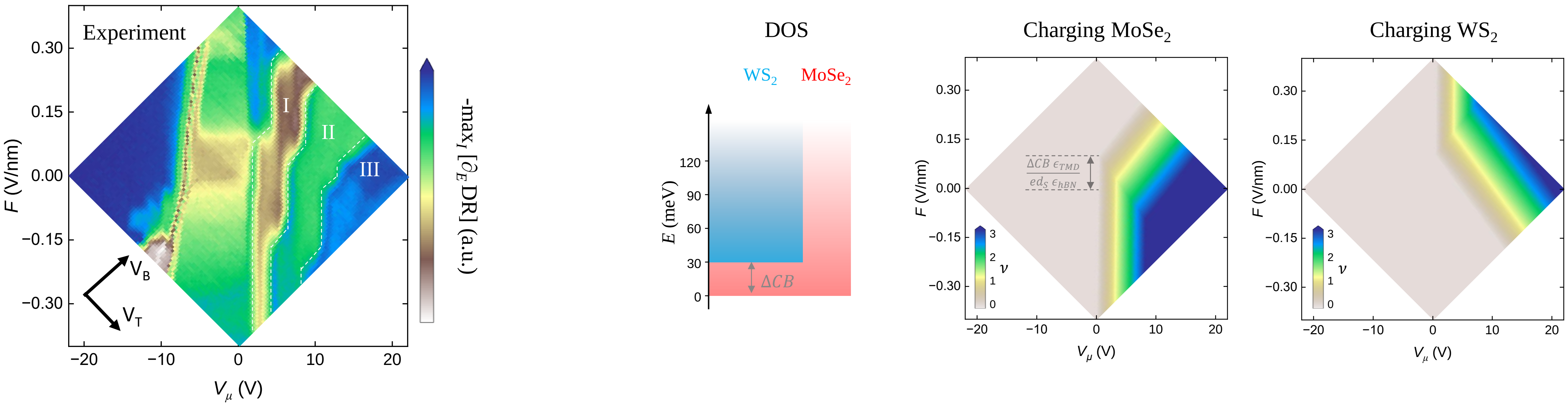

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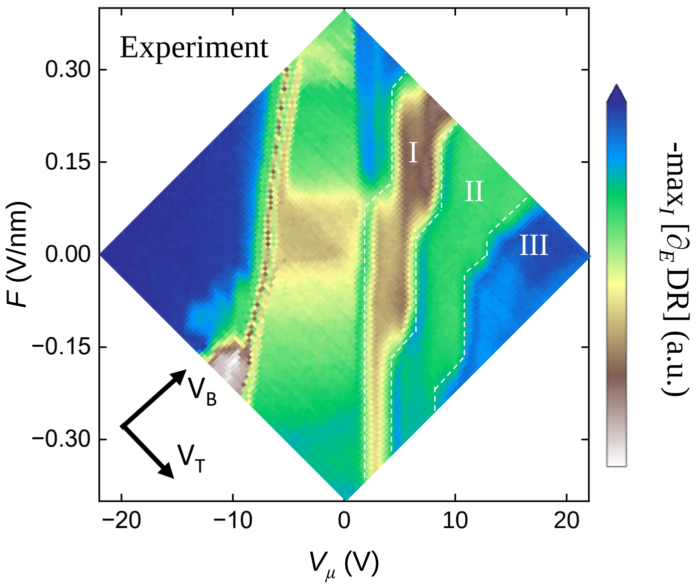

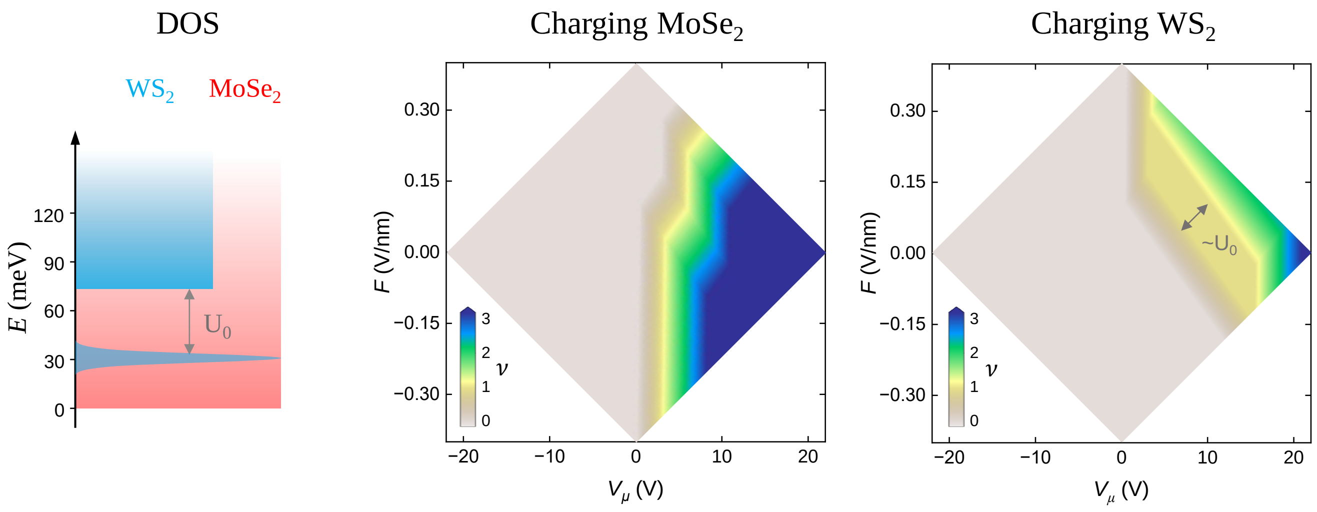

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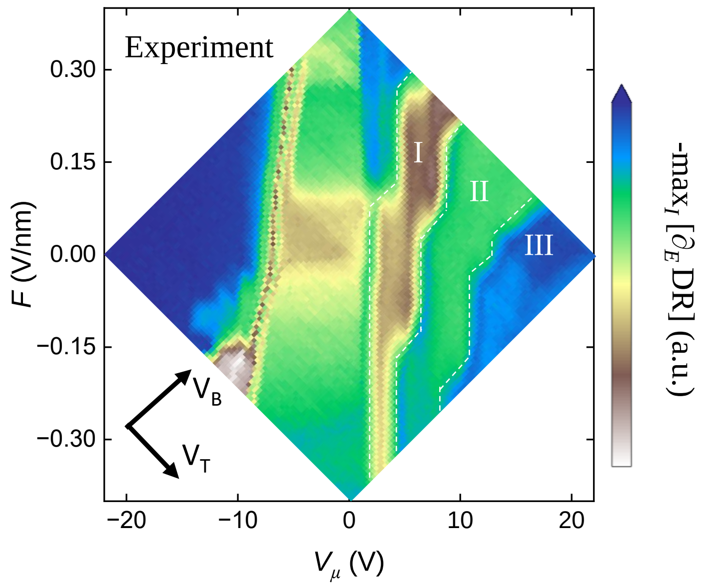

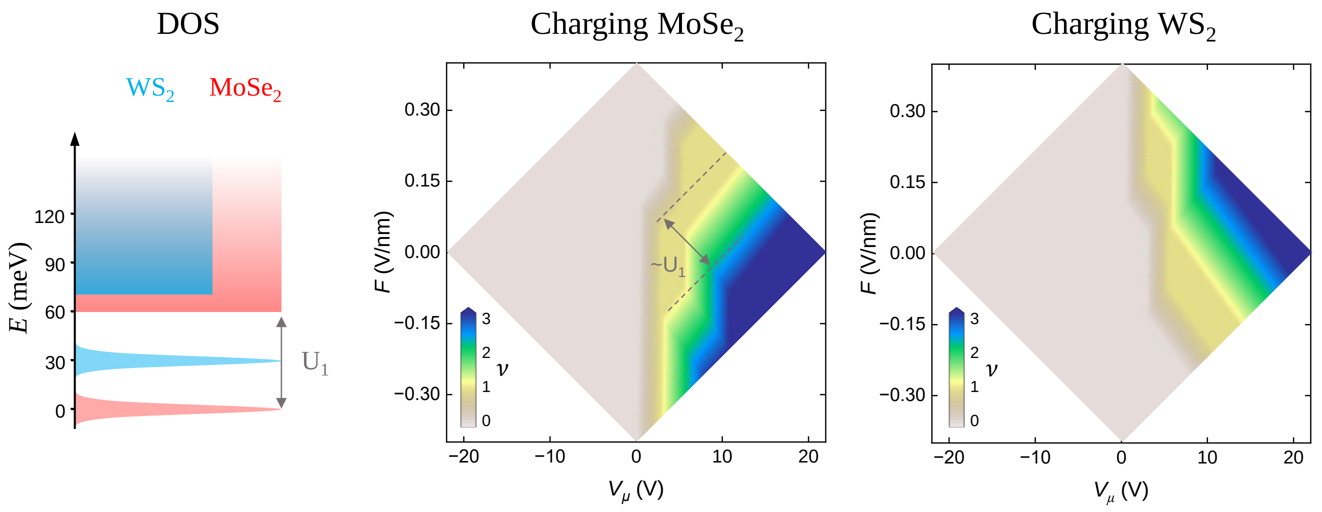

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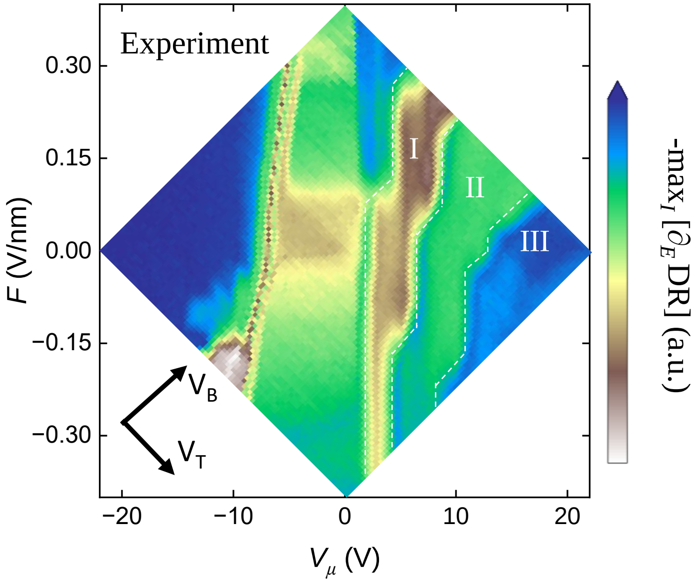
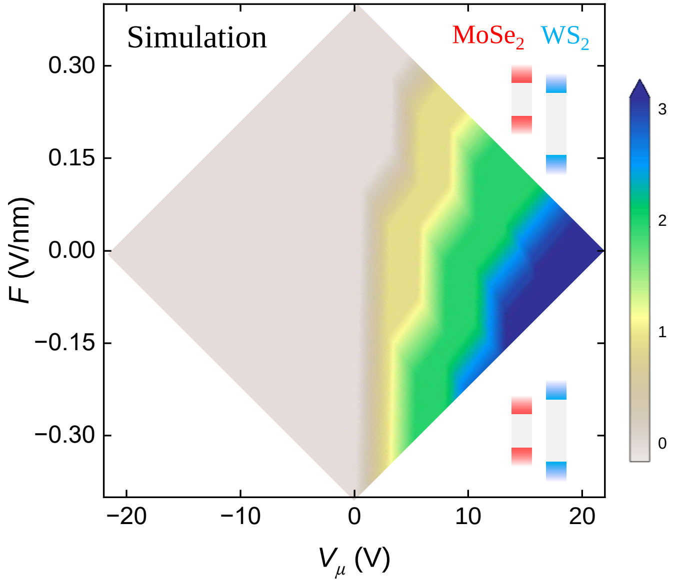
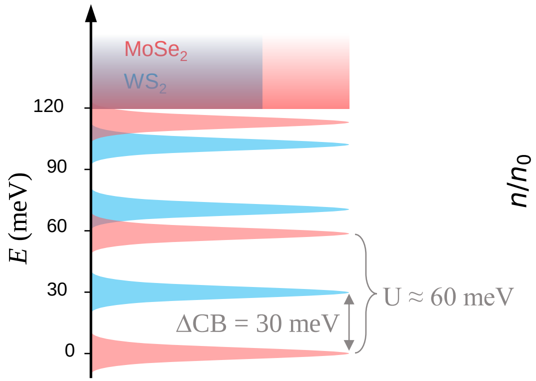
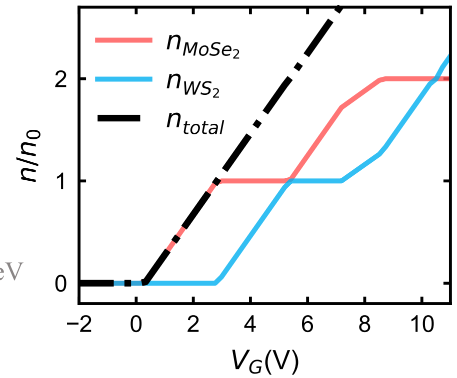
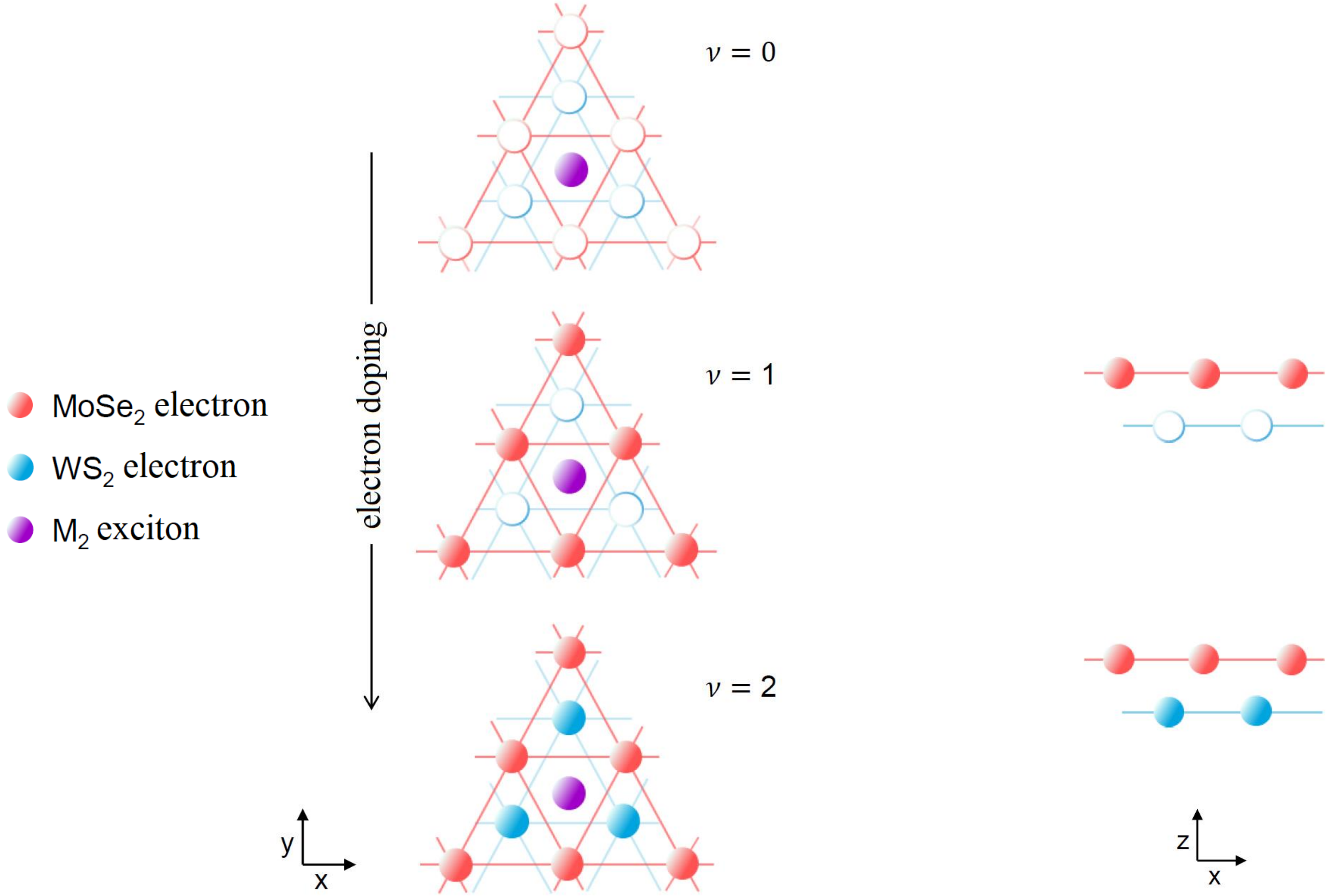




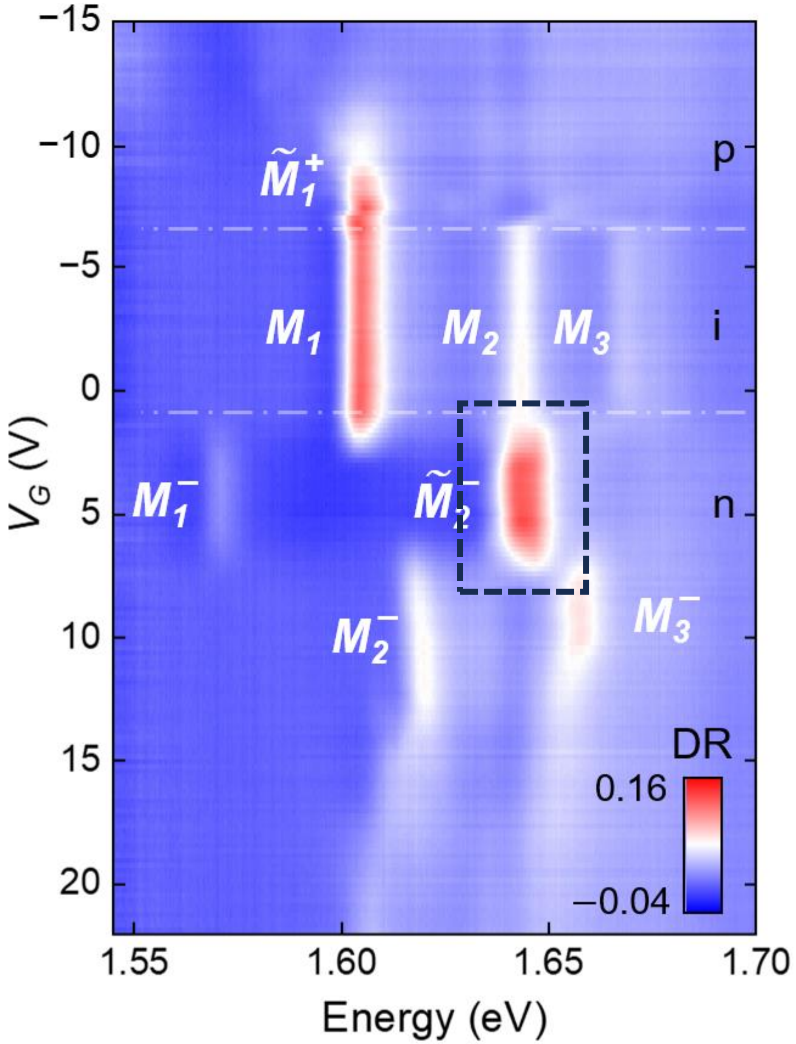


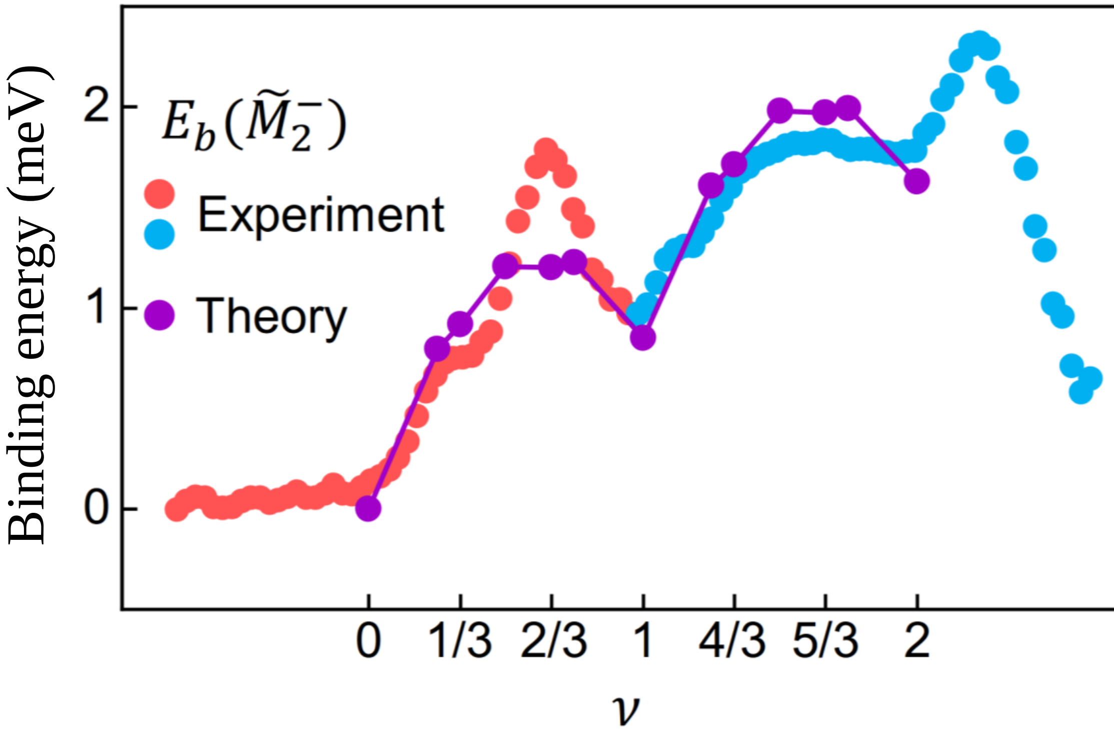


Layer-by-layer charging: schematics



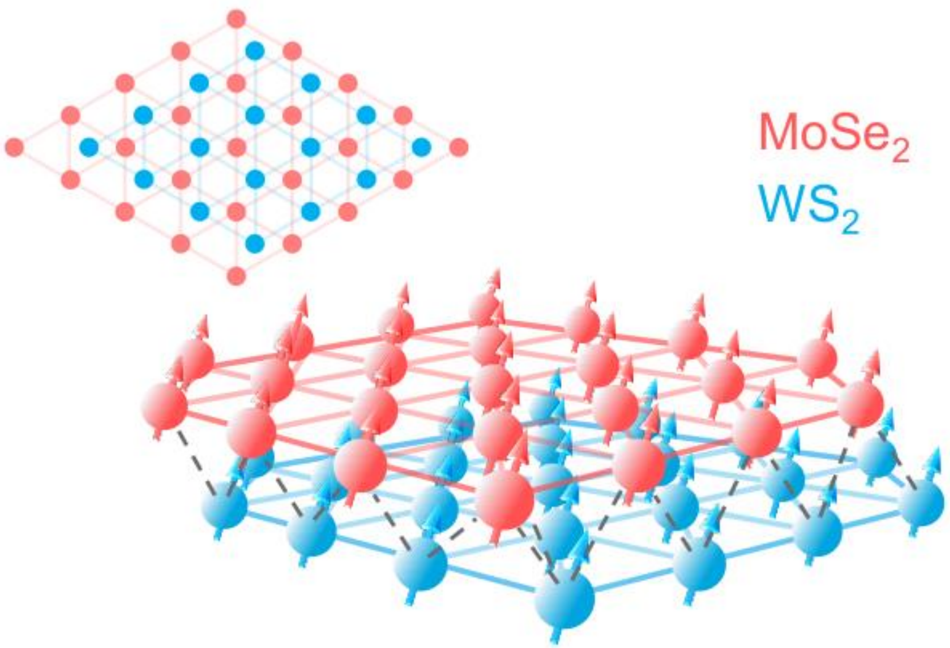
Trion binding energy

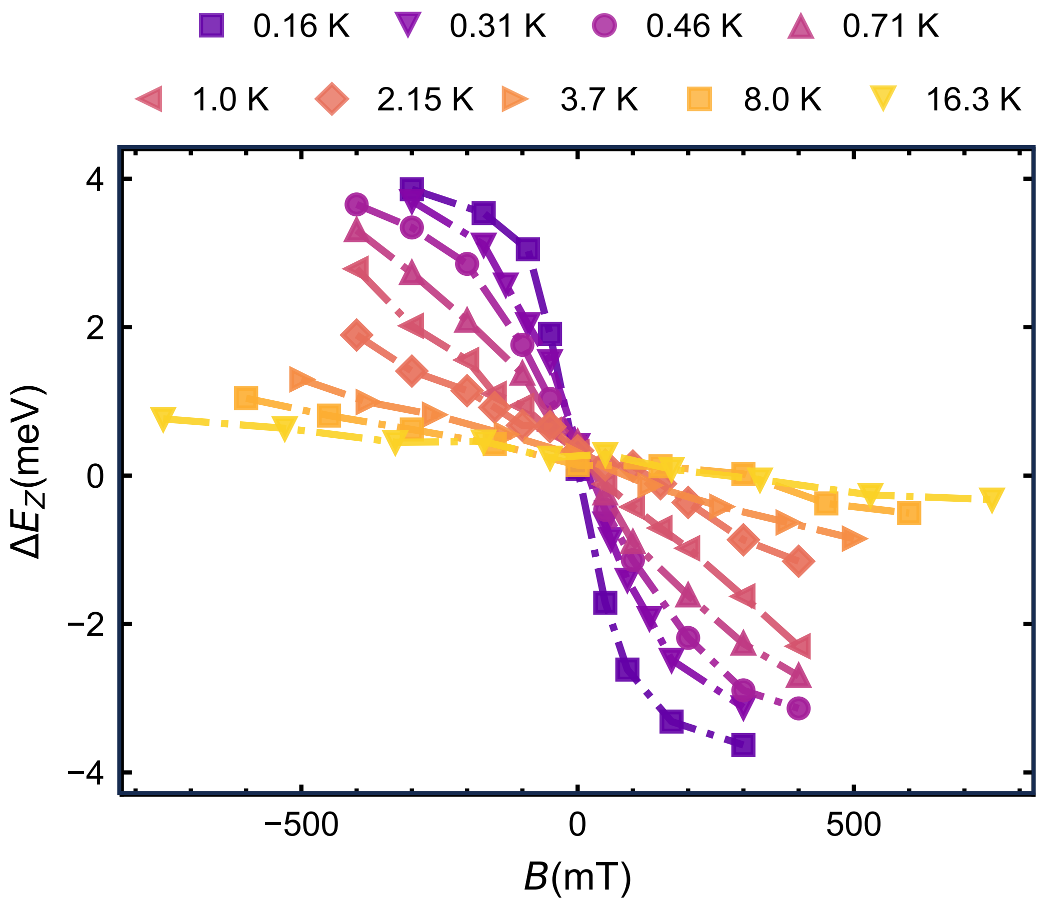




Spin-susceptibility sensed by the moiré exciton

Spin-susceptibility measured by the exciton Landé g-factor (Zeeman shift) of the moiré exciton





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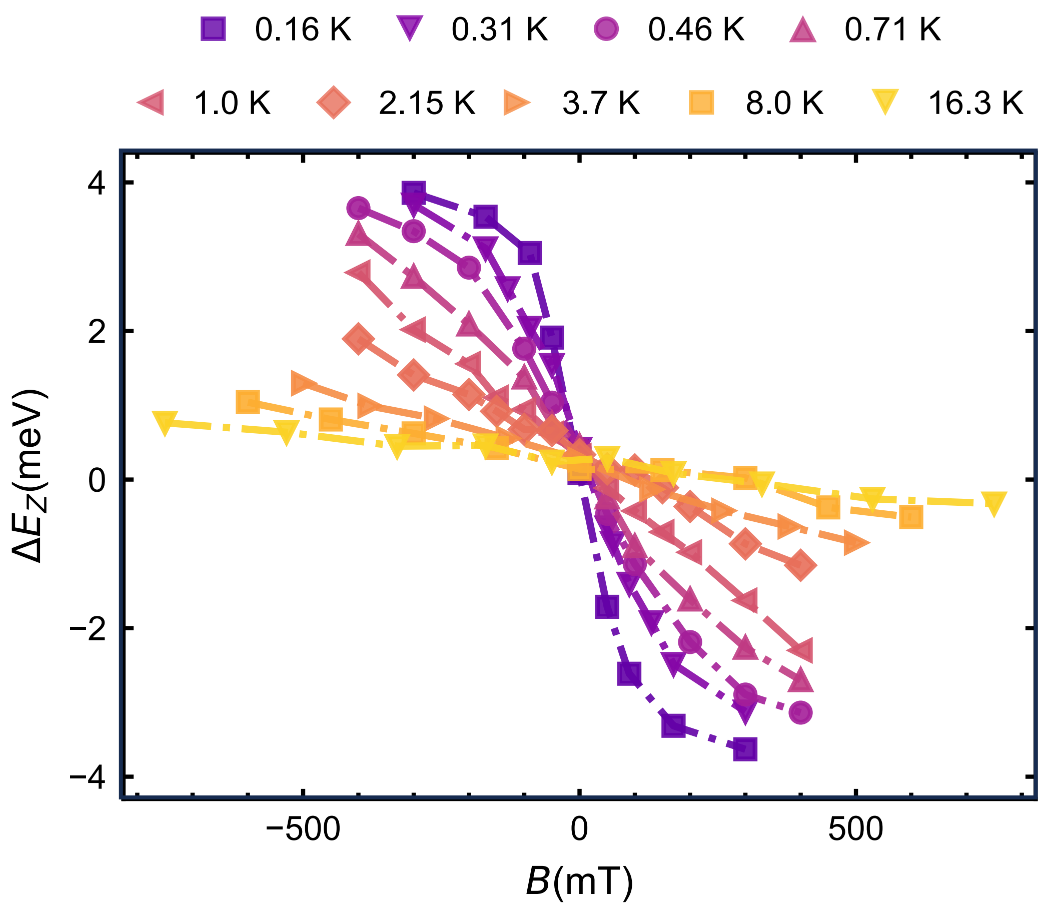
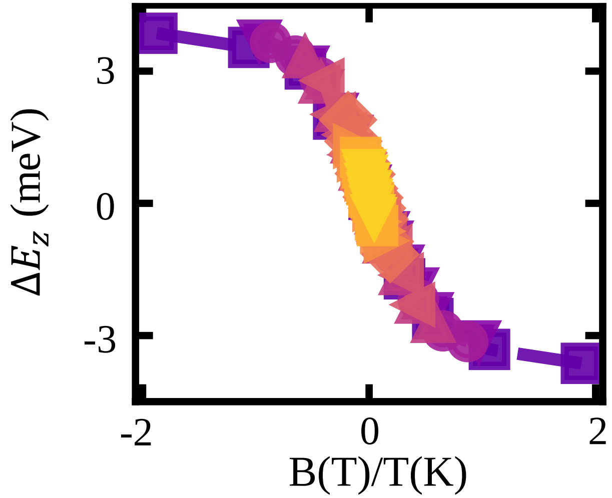
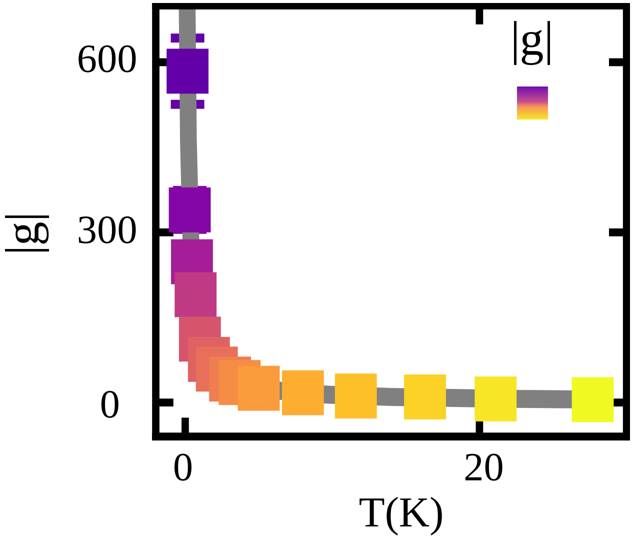
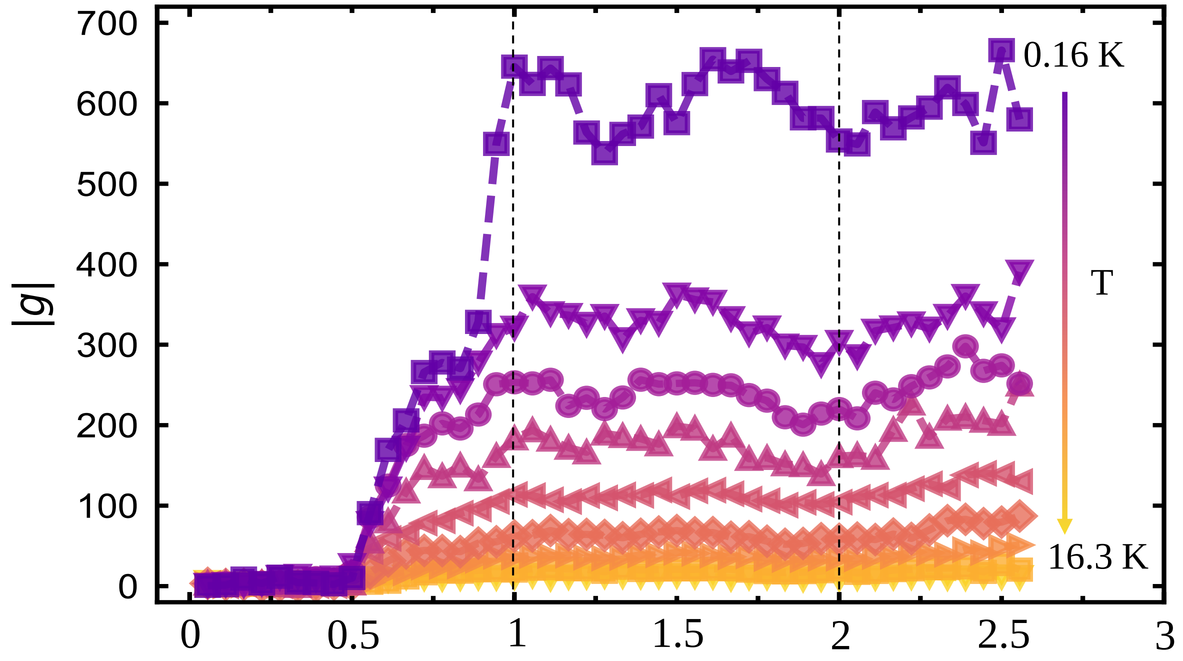
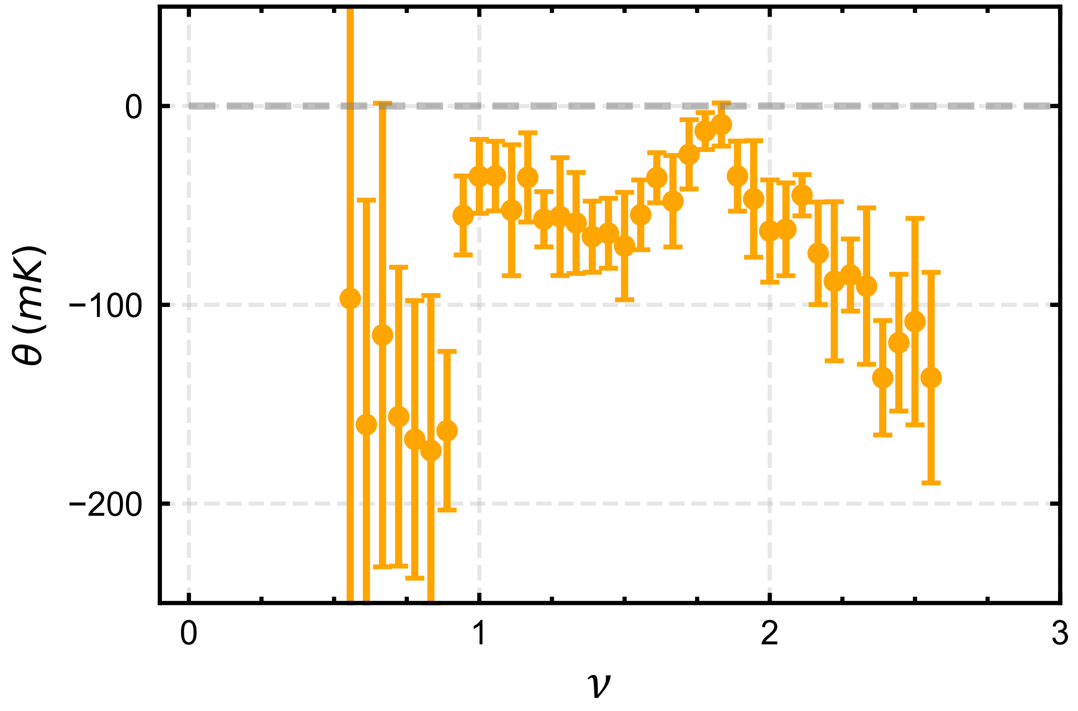






Correlated magnetism as a function of charging





Curie-Weiss law: $\chi = C/(T - \theta)$

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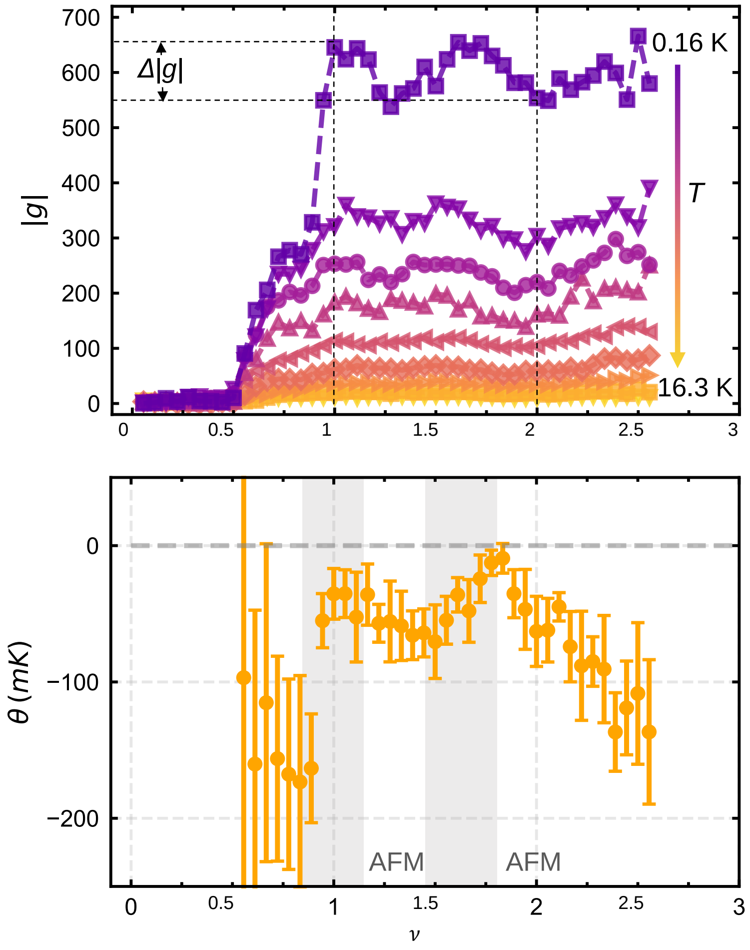

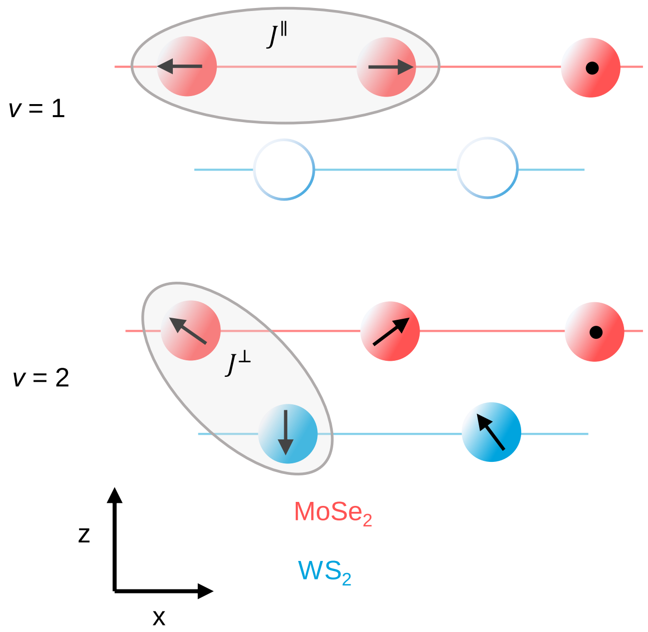

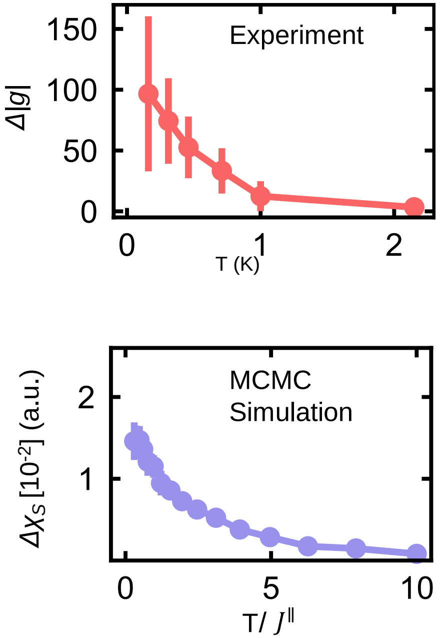

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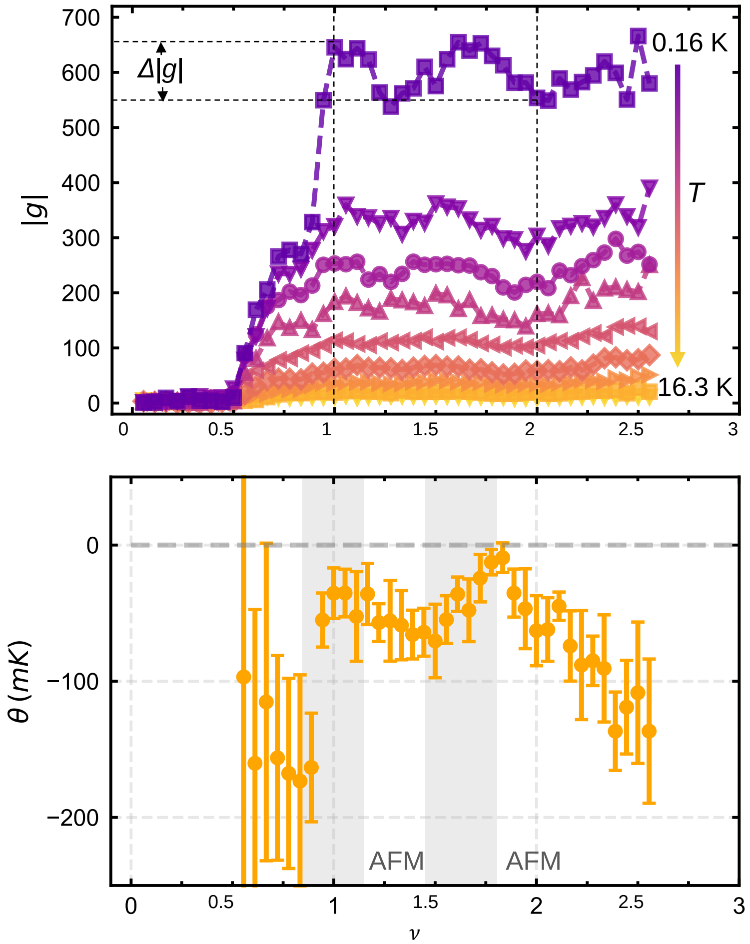

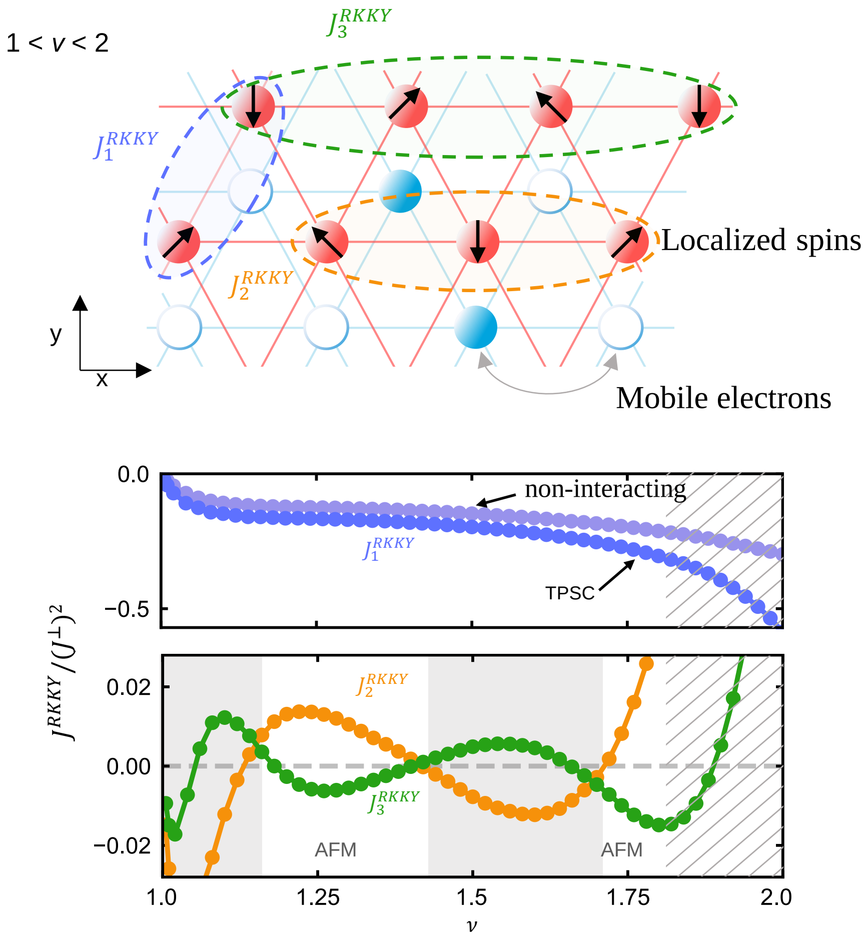

Ruderman-Kittel-Kasuya-Yosida (RKKY) magnetism

Summary

- Staggered bilayer triangular lattice exhibiting Hubbard model physics
- Layer-by-layer charging sequence, firstly filling of one electron per moiré cell in $MoSe_2$, then the same in WS_2, and so on
- Experimental determination of conduction band offset (~ 30 meV) and on-site Coulomb repulsion (~ 60 meV)
- Transition from type-I to type-II band-alignment by out-of-plane electric field
- Spin-correlations on the vertically offset bilayer lattice, weak antiferromagnetic coupling, RKKY magnetism

arXiv:2404.05494

Acknowledgements

Experiment

Borislav Polovnikov, Johannes Scherzer, Anvar Baimuratov & Alexander Högele

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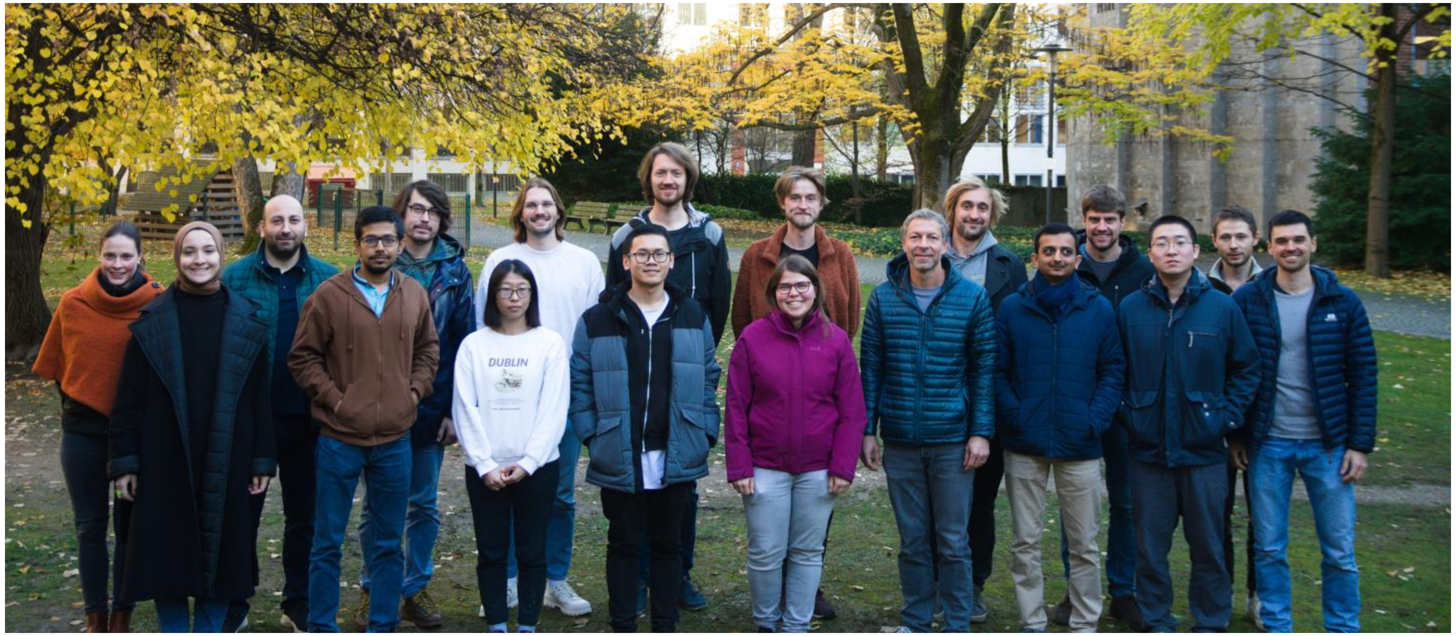
Many-body theory

Henning Schlömer, Annabelle Bohrdt, Fabian Grusdt



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