Quantum transport simulations for twistronic and spintronic 2D materials

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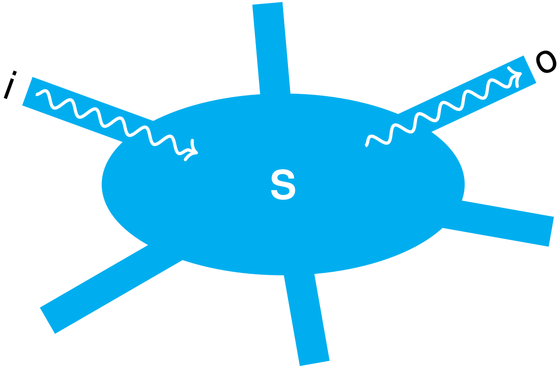
28 December 2024

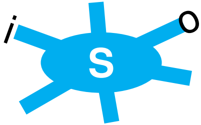
Real-space Green's function method: Recipe



(S: scattering region, i: incoming lead, o: outgoing lead)

Real-space Green's function method: Recipe

See Datta, S., *Electronic Transport in Mesoscopic Systems*, Cambridge University Press, Cambridge, 1995 for more.



Brief summary of the recipe (if N sites, single-orbital):

$$H_0 = [\cdots]_{N\times N} \qquad \text{(clean tight-binding Hamiltonian)}$$

$$U = [\cdots]_{N\times N} \qquad \text{(onsite energy)}$$

$$\Sigma_p(E) = [\cdots]_{N\times N} \qquad \text{(self-energy at energy } E \text{ for lead } p\text{)}$$

$$H(E) = H_0 + U + \sum_p \Sigma_p(E) \qquad \text{(effective Hamiltonian)}$$

$$G_R(E) = [E\mathbb{1} - H]^{-1} \qquad \text{(retarded Green's function at energy } E\text{)}$$

$$\Gamma_p(E) = -2\,\mathrm{Im}\Sigma_p(E) \qquad \text{(broadening matrix at energy } E \text{ for lead } p\text{)}$$

$$T_{o\leftarrow i}(E) = \mathrm{Tr}\left[\Gamma_o(E)G_R(E)\Gamma_i(E)G_R^\dagger(E)\right] \qquad \text{(transmission from } i \text{ to } o\text{)}$$

Revisiting an old experiment

From van Wees, B. J. et al., Phys. Rev. Lett. **60** (1988) 848:

VOLUME 60, NUMBER 9 PHYSICAL REVIEW LETTERS 29 FEBRUARY 1988

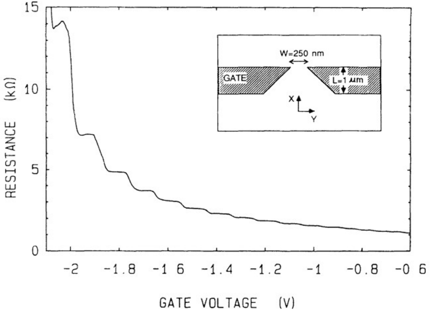


FIG. 1. Point-contact resistance as a function of gate voltage at 0.6 K. Inset: Point-contact layout.

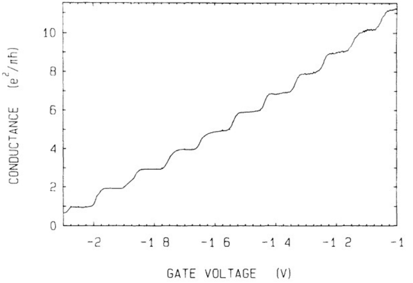
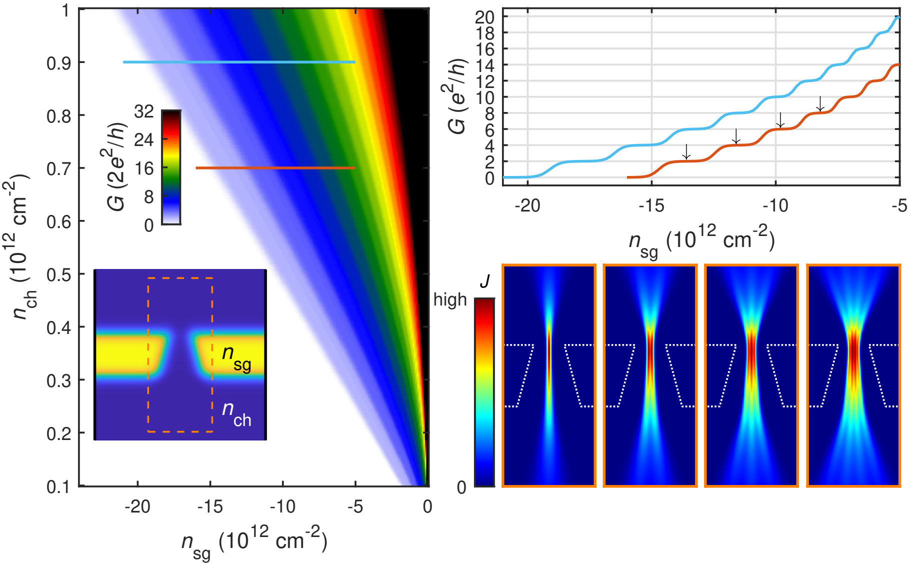


FIG. 2. Point-contact conductance as a function of gate voltage, obtained from the data of Fig. 1 after subtraction of the lead resistance. The conductance shows plateaus at multiples of $e^2/\pi\hbar$.

Imaging local current & charge densities



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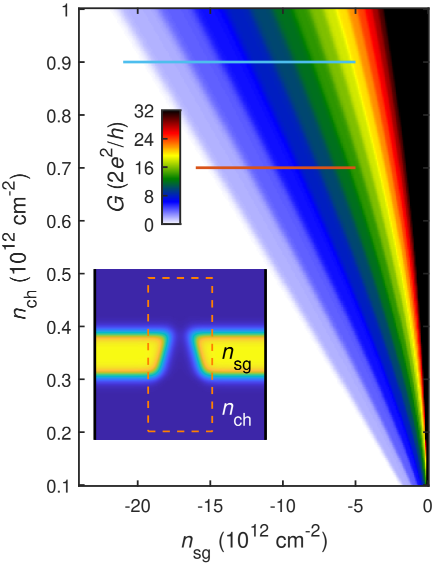

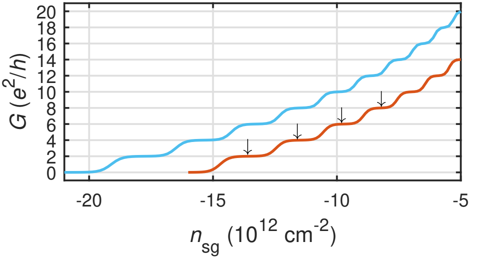

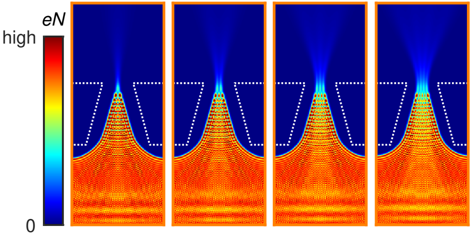

Some recent highlights of my group

- Garcia-Ruiz, A. and Liu, M.-H., Nano Letters **24** (2024) 16317
  - Twisted Bilayer MoS_2 under Electric Fields: A System with Tunable Symmetry
- Kang, W.-H. et al., Phys. Rev. Lett. **133** (2024) 216201
  - Magnetotransport and Spin-Relaxation Signatures of the Radial Rashba and Dresselhaus Spin-Orbit Coupling in Proximitized Graphene
- Chen, S.-C., Mreńca-Kolasińska, A., and Liu, M.-H., Phys. Rev. Appl. **22** (2024) 024039
  - Four-band effective square-lattice model for Bernal-stacked bilayer graphene
- Rao, Q. et al., Nature Communications **14** (2023)
  - Ballistic transport spectroscopy of spin-orbit-coupled bands in monolayer graphene on WSe_2
- Rickhaus, P. et al., Science Advances **6** (2020)
  - The electronic thickness of graphene

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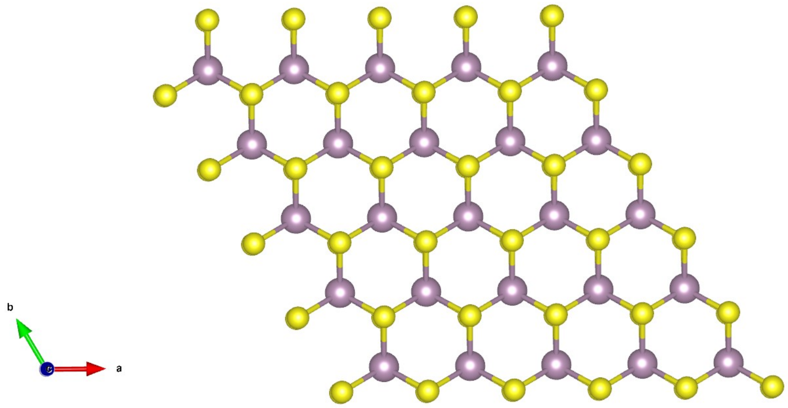
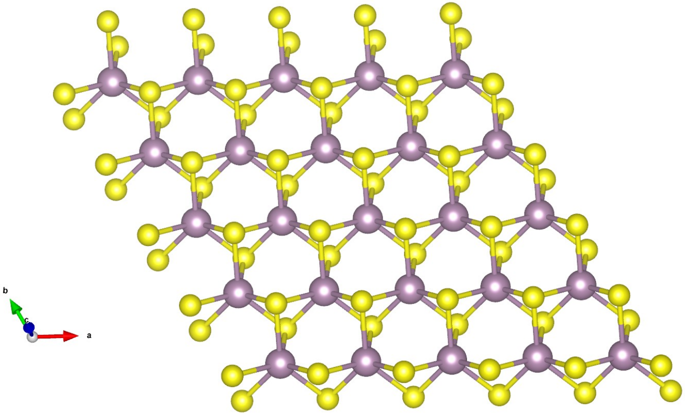
The MoS_2 monolayer



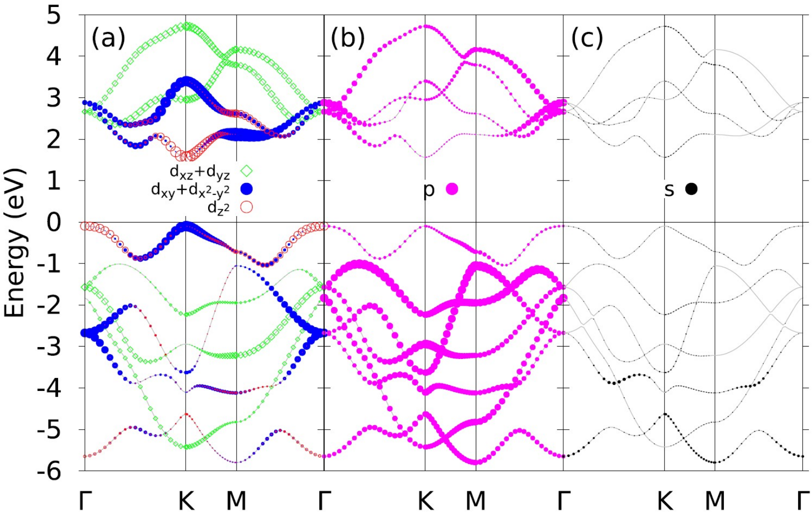
(Top view)

The MoS_2 monolayer



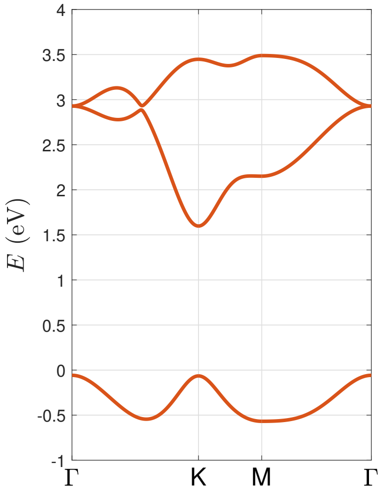
(Slightly tilted)

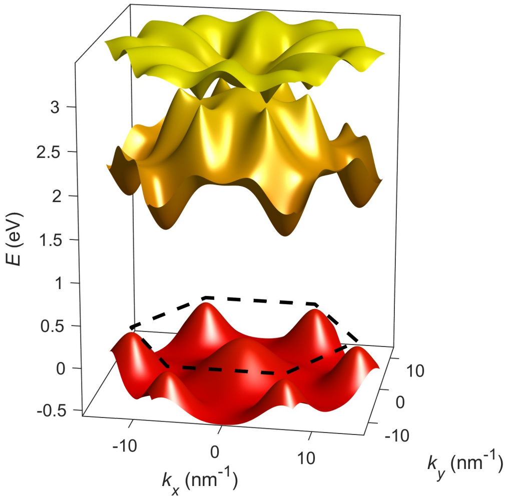
Band structure of MoS_2 monolayer based on DFT†



†Liu, G.-B., Shan, W.-Y., Yao, Y., Yao, W., and Xiao, D., Physical Review B **88** (2013)

Following the 3-band model†





† Liu, G.-B., Shan, W.-Y., Yao, Y., Yao, W., and Xiao, D., Physical Review B **88** (2013)

Finite-difference approximation

For a 1D Schrödinger equation,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right]\psi(x)=E\psi(x)\ ,$$

we may[1]:

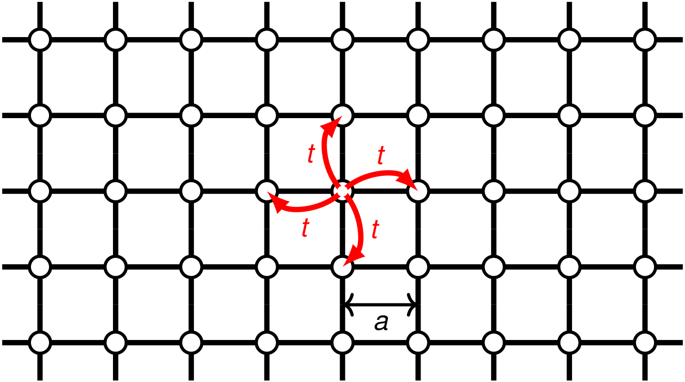
$$\frac{d}{dx}\psi(x)\approx\frac{\psi(x+\frac{a}{2})-\psi(x-\frac{a}{2})}{a}$$
$$\frac{d^2}{dx^2}\psi(x)\approx\frac{\psi(x+a)+\psi(x-a)-2\psi(x)}{a^2}$$

Therefore:

$$\begin{aligned}-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)&\approx-\frac{\hbar^2}{2ma^2}\left[\psi(x+a)+\psi(x-a)-2\psi(x)\right]\\&=-t\left[\psi(x+a)+\psi(x-a)-2\psi(x)\right]\end{aligned}$$

[1] Datta, S., *Electronic Transport in Mesoscopic Systems*, Cambridge University Press, Cambridge, 1995

Finite-difference-based square lattice



$$H = \sum_{\langle i,j \rangle} t c_i^\dagger c_j + \sum_n U_i c_i^\dagger c_i \ , \qquad t = \begin{pmatrix} t_e & 0 \\ 0 & t_h \end{pmatrix}$$

Two-band effective mass model for MoS_2

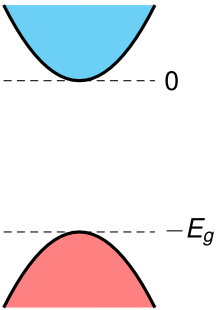
$$H = \sum_{\langle i,j \rangle} t c_i^\dagger c_j + \sum_n U_i c_i^\dagger c_i$$

$$t = \begin{pmatrix} t_e & 0 \\ 0 & t_h \end{pmatrix} , \quad t_e = -\frac{\hbar^2}{2m_e^* a^2} , \quad t_h = \frac{\hbar^2}{2m_h^* a^2}$$

$$U_i = \begin{pmatrix} U_{i,e} & 0 \\ 0 & U_{i,h} \end{pmatrix}$$

$$U_{i,e} = -4t_e + V(\mathbf{r}_i)$$

$$U_{i,h} = -4t_h - E_g + V(\mathbf{r}_i)$$

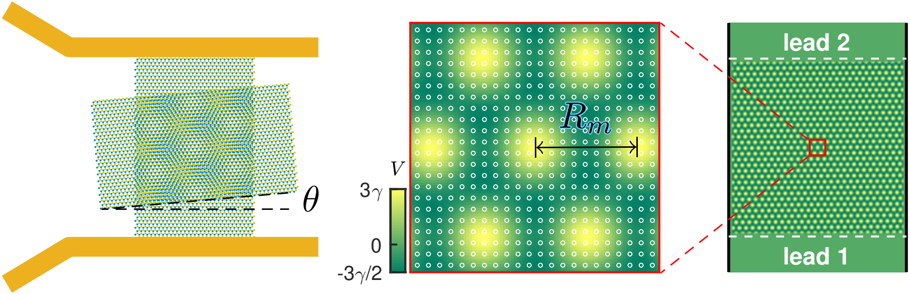


Using effective masses[a] $m_e^* = 0.4625$, $m_h^* = 0.5659$ and adopting $a = 2\,\text{nm}$, hopping parameters are:

$$t_e = -0.0206\,\text{eV} , \quad t_h = 0.0168\,\text{eV}$$

[a] Fang, S. et al., Phys. Rev. B **92** (2015) 205108

A fun calculation done nearly 2 years ago

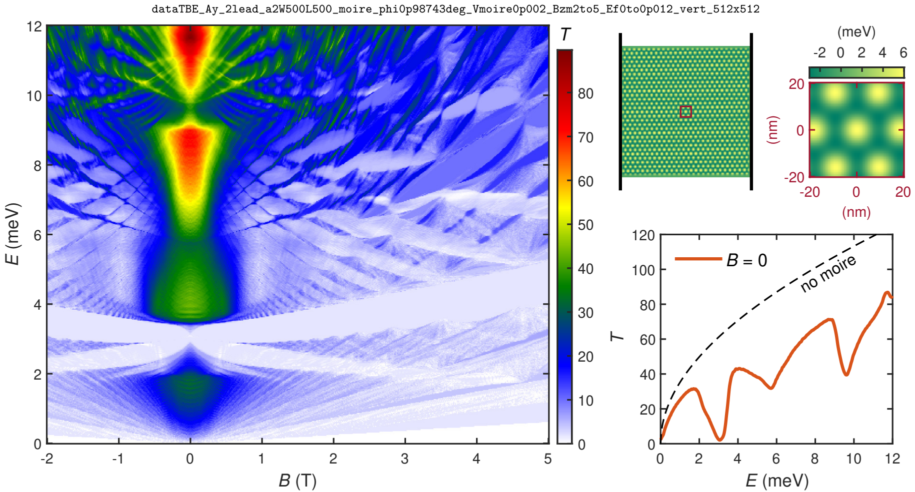


We consider

- $\theta \approx 1^\circ \implies R_m \approx 18.47\,\text{nm}$
- $\gamma = 2\,\text{meV}$
- $500\,\text{nm} \times 500\,\text{nm}$

$$V(\mathbf{r}) = \gamma \sum_{j=1}^{3} \cos(\mathbf{G}_j \cdot \mathbf{r})$$

A fun calculation done nearly 2 years ago



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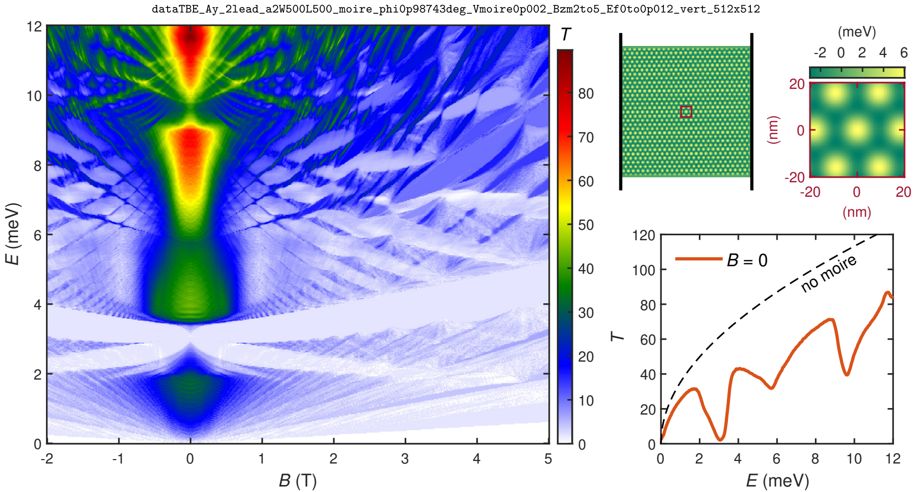
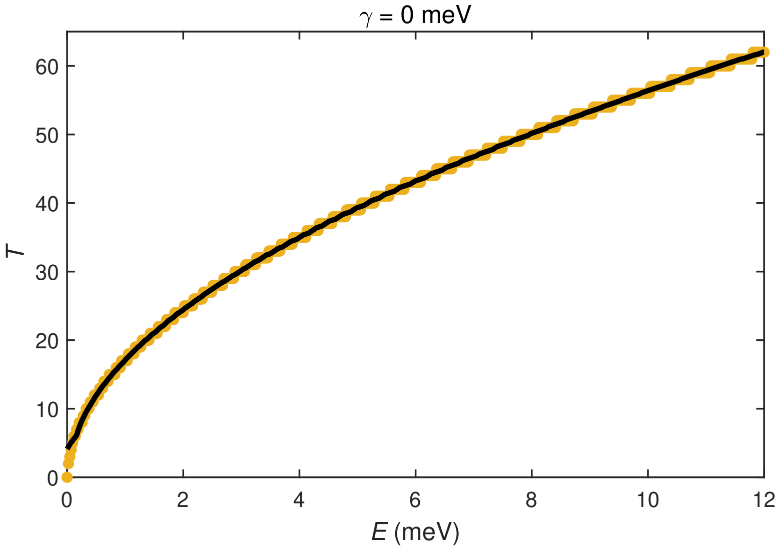


What about other values of γ?

Test calculations: Coupling strength dependence



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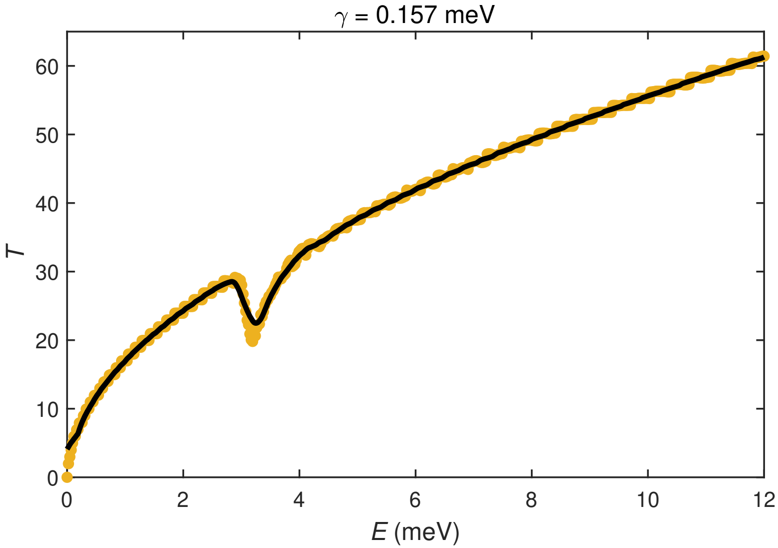

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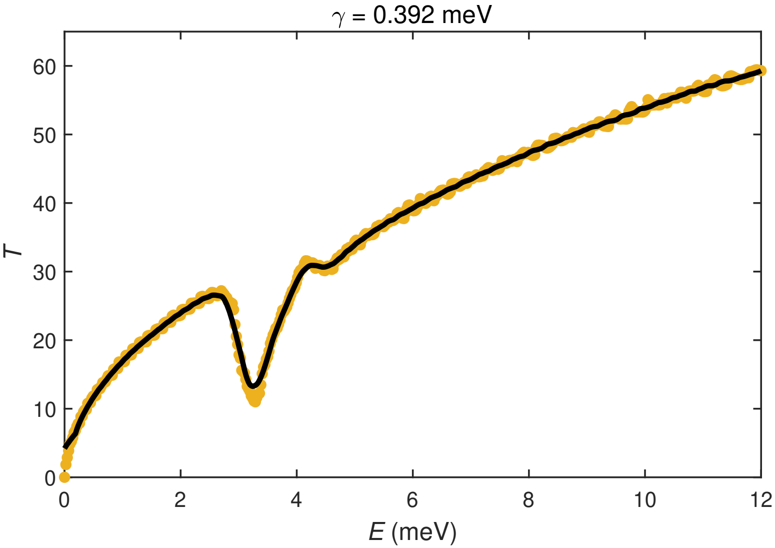

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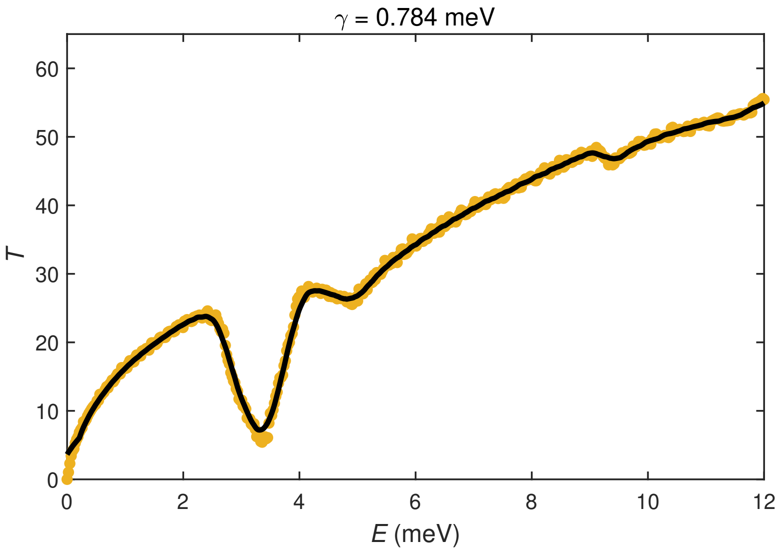

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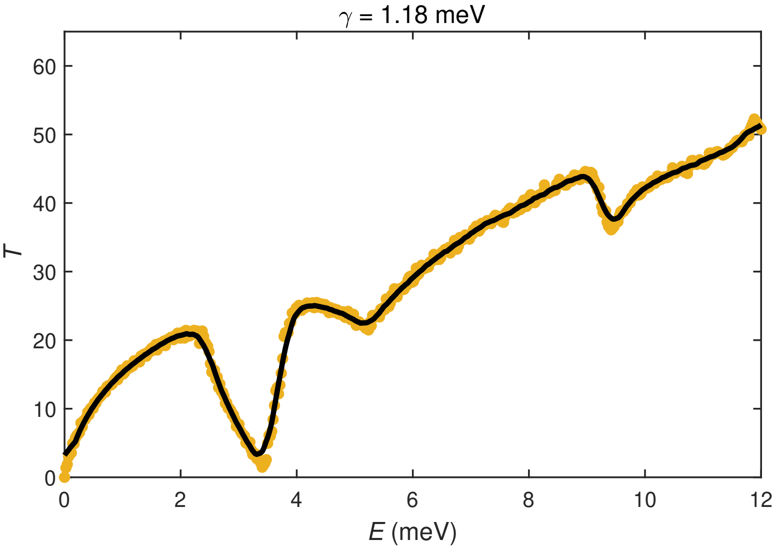

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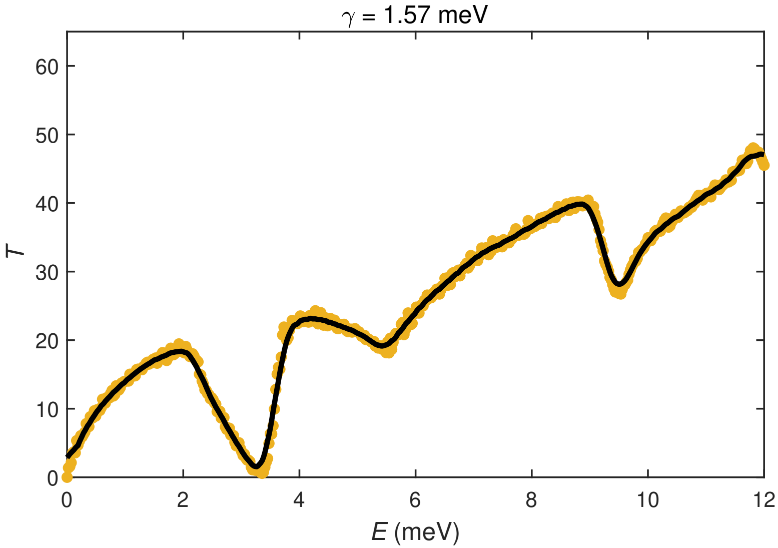

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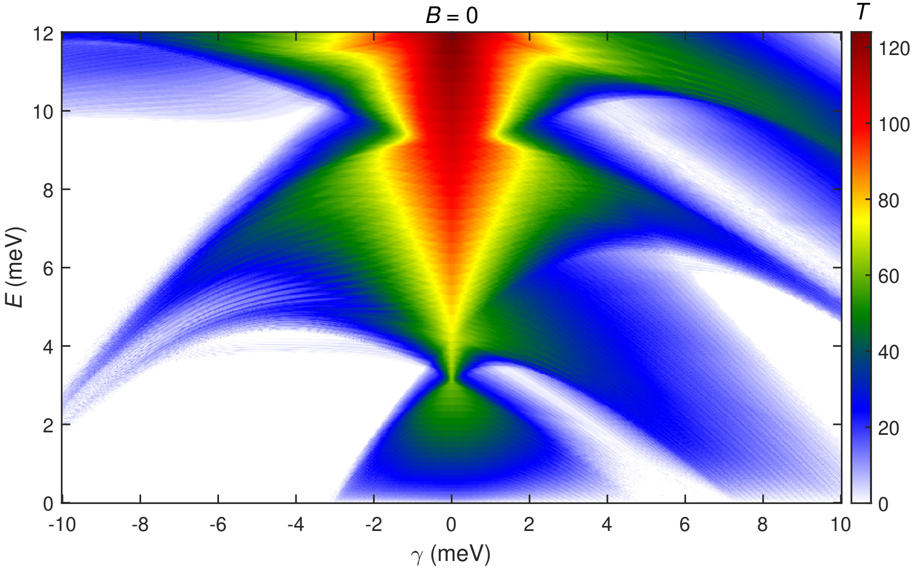
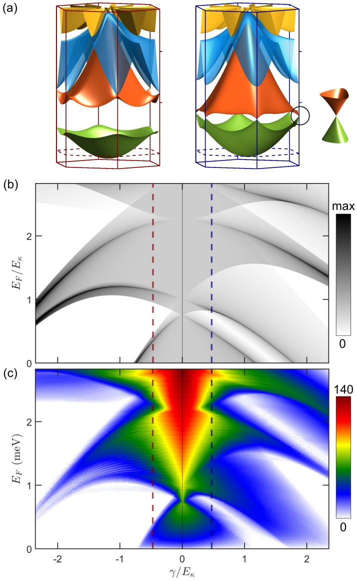


What's going on here?



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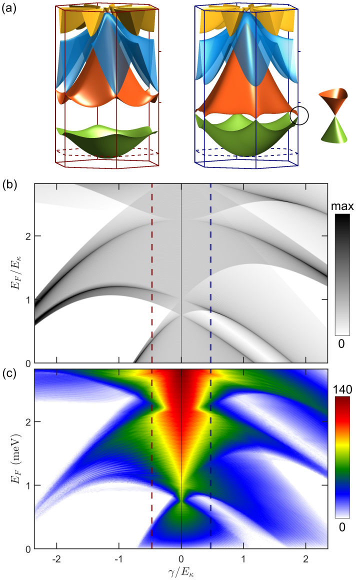

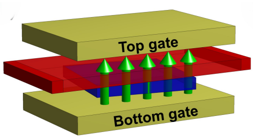

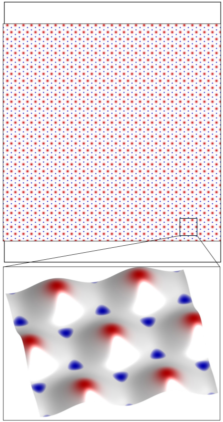

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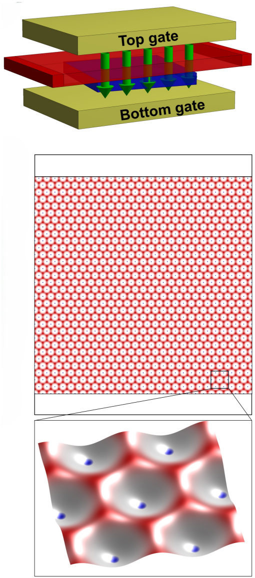
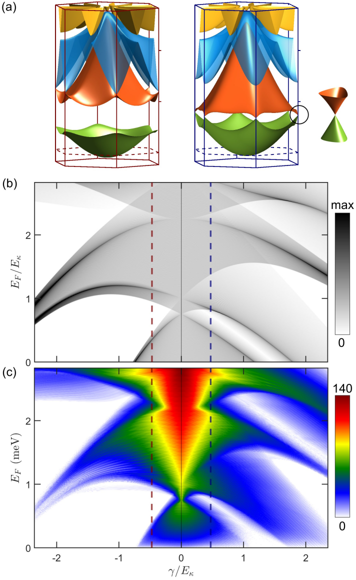
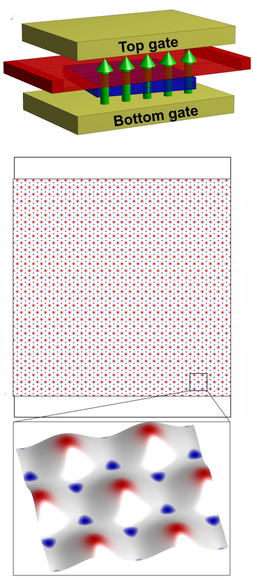
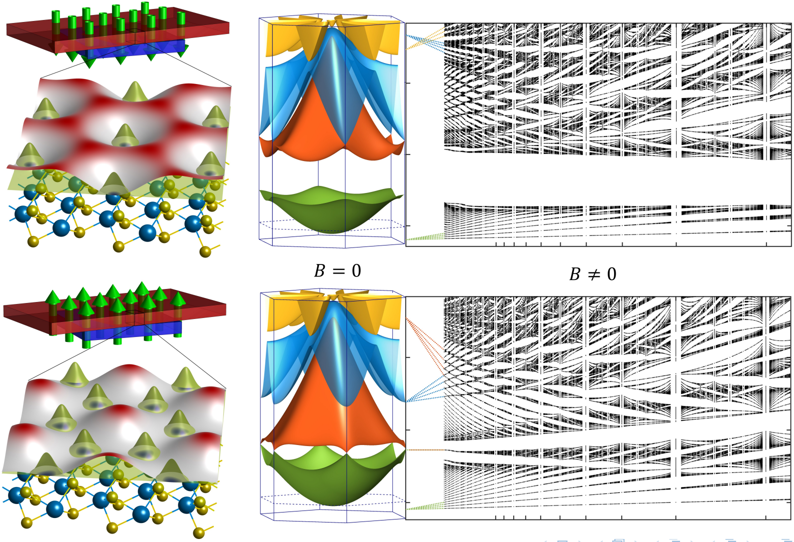






Twisted bilayer MoS_2 with tunable symmetry

Garcia-Ruiz, A. and Liu, M.-H., Nano Letters **24** (2024) 16317



Acknowledgments

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- Denis Kochan, Andreas Costa, Michael Barth for the radial Rashba paper
- Qing Rao and Dong-Keun Ki for the spin-TMF paper
- Financial: National Science and Technology Council of Taiwan
- Computational: National Center for High-performance Computing