2D Layered Materials: Ab-initio Wannier Tight-Binding Hamiltonian Approach

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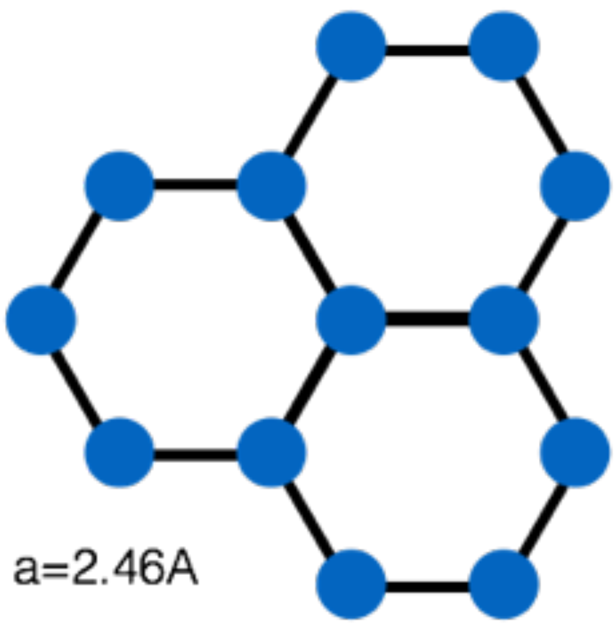
2D Layered Materials

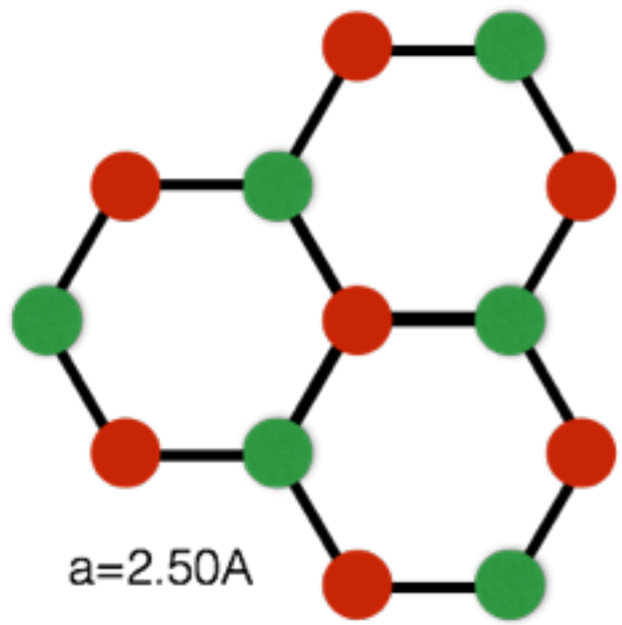
Graphene



Semimetal

- Relativistic linear Dirac dispersion at K valleys
- Inversion symmetry
- Mechanical strength

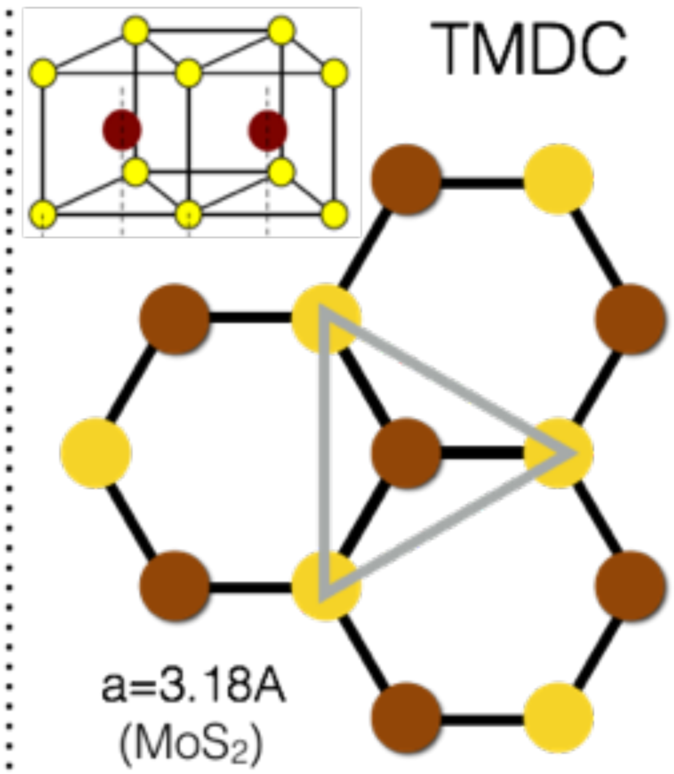
hBN



Insulator

- Broken inversion symmetry
- Used to encapsulate graphene
- Stability
- Large band gap

TMDC



Semiconductor

- MX_2, M=Mo/W, X=S/Se
- Broken inversion symmetry
- Direct band gap 1-2 eV at K valleys
- Spin-orbit coupling

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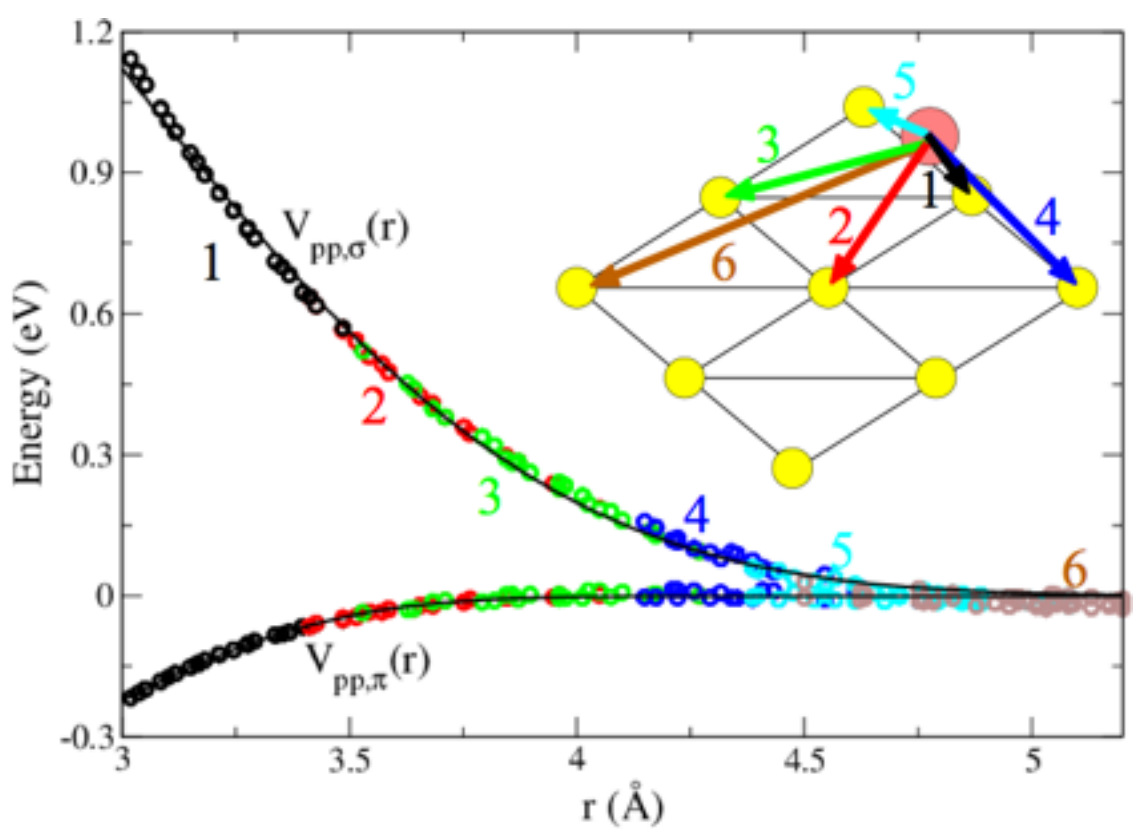
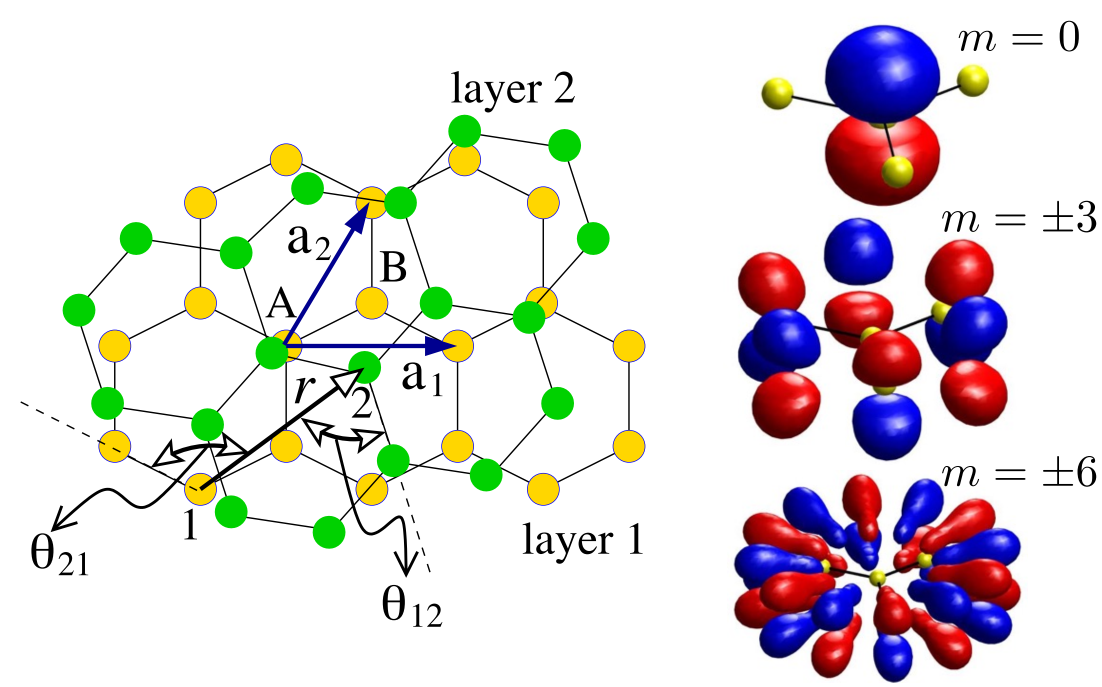
Outline

- Electrons in solids and non-interacting electron approximation
- Ab-initio tight-binding hamiltonian from Wannier transformation based on density functional theory calculations
- Modeling for 2D layered material heterostructures and example with twisted bilayer graphene
- Wannier construction and topological obstructions



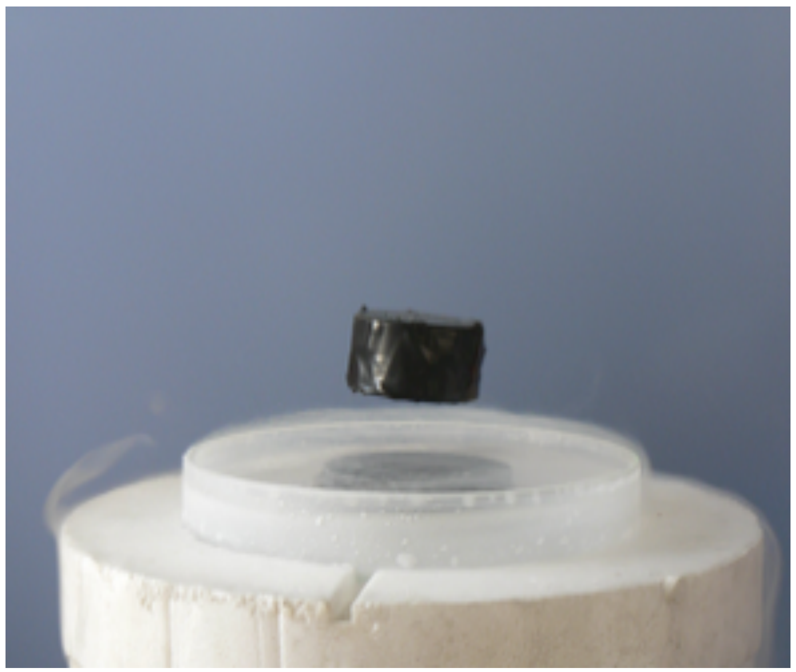
TMDC interlayer coupling



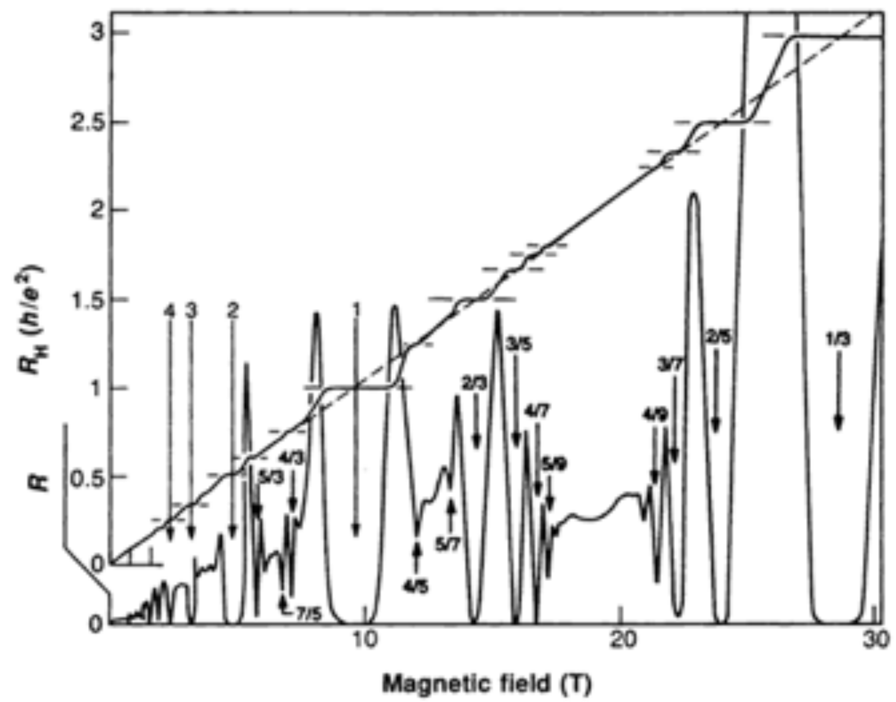
graphene interlayer coupling

Electrons in Solids

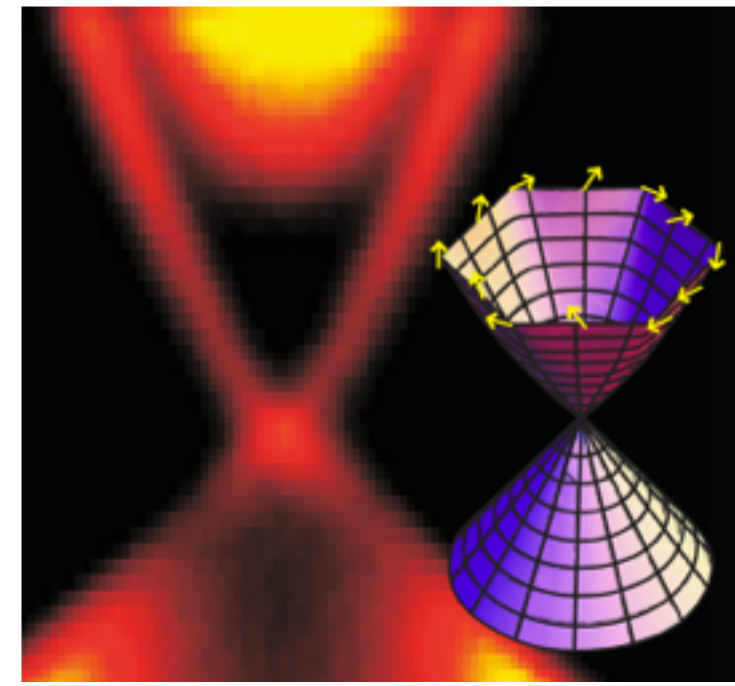
High temperature superconductivity



Fractional quantum Hall



Topological Insulator



- Strongly correlated phases
- Topological phases
- Anyonic statistics
- Spin liquids

Or simply behave as non-interacting electrons (Fermi liquid theory) !

Ref: **P. W. Anderson, More is different,** Science, New Series, Vol. 177, pp 39

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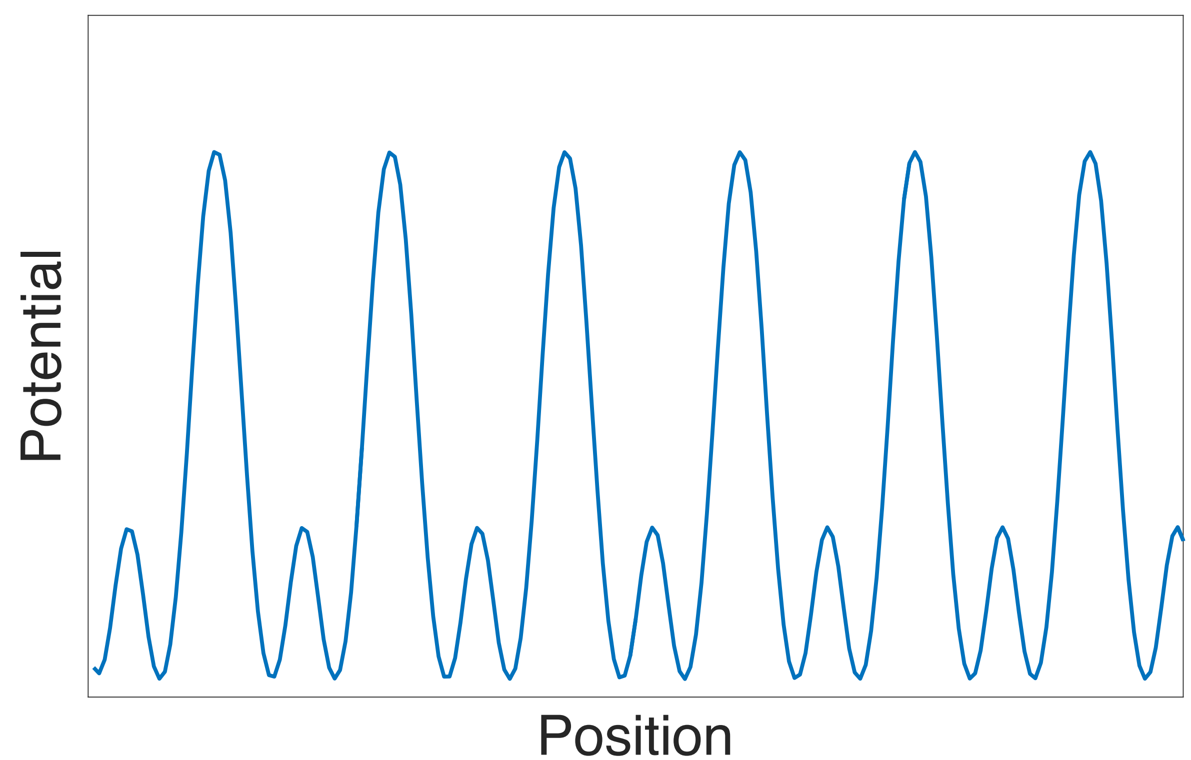
Electrons in Solids

Non-interacting Hamiltonian

$$-\frac{\hbar^2}{2m}\partial_x^2\Psi(x) + V(x)\Psi(x) = E\Psi(x)$$

Periodic potential

$$V(x+a) = V(x)$$



Ref: Efthimios Kaxiras, Atomic and Electronic Structure of Solids

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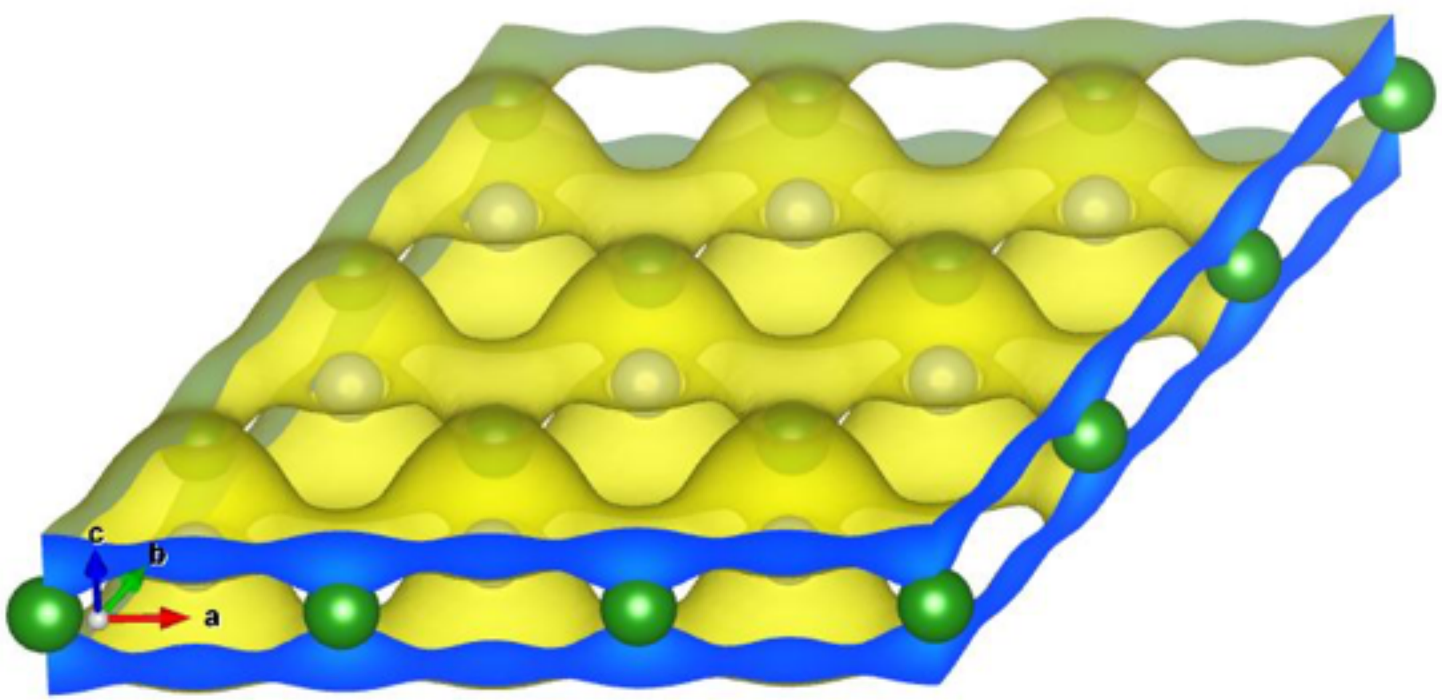
Electrons in Solids



Example: pz bonding orbital for hexagonal boron nitride layer

$$\Psi(x+a) = e^{ika}\Psi(x)$$

- Wavefunction satisfies twist boundary condition and is extended in space
- Bands are classfied into band index n and crystal momentum label k (diagonal hamiltonian).

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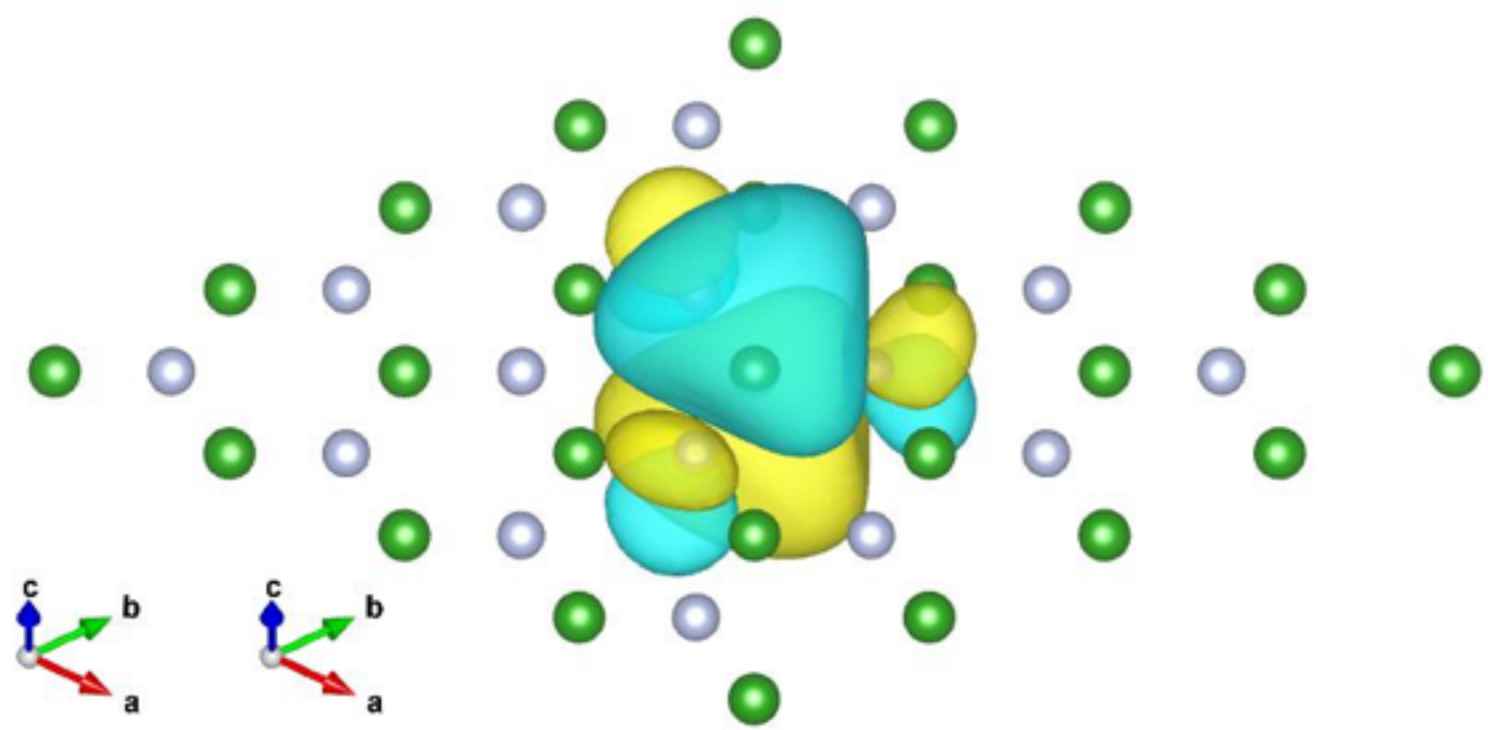
Wannier Functions: Localized Basis

$$|\vec{R}> = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} |\vec{k}> e^{-i\vec{k}\vec{R}} dk$$



Example: Wannier pz orbital for hexagonal boron nitride layer

- Fourier transform from extended Bloch waves to localized Wannier basis
- The hamiltonian is transformed into tight-binding form with short-range hoppings.

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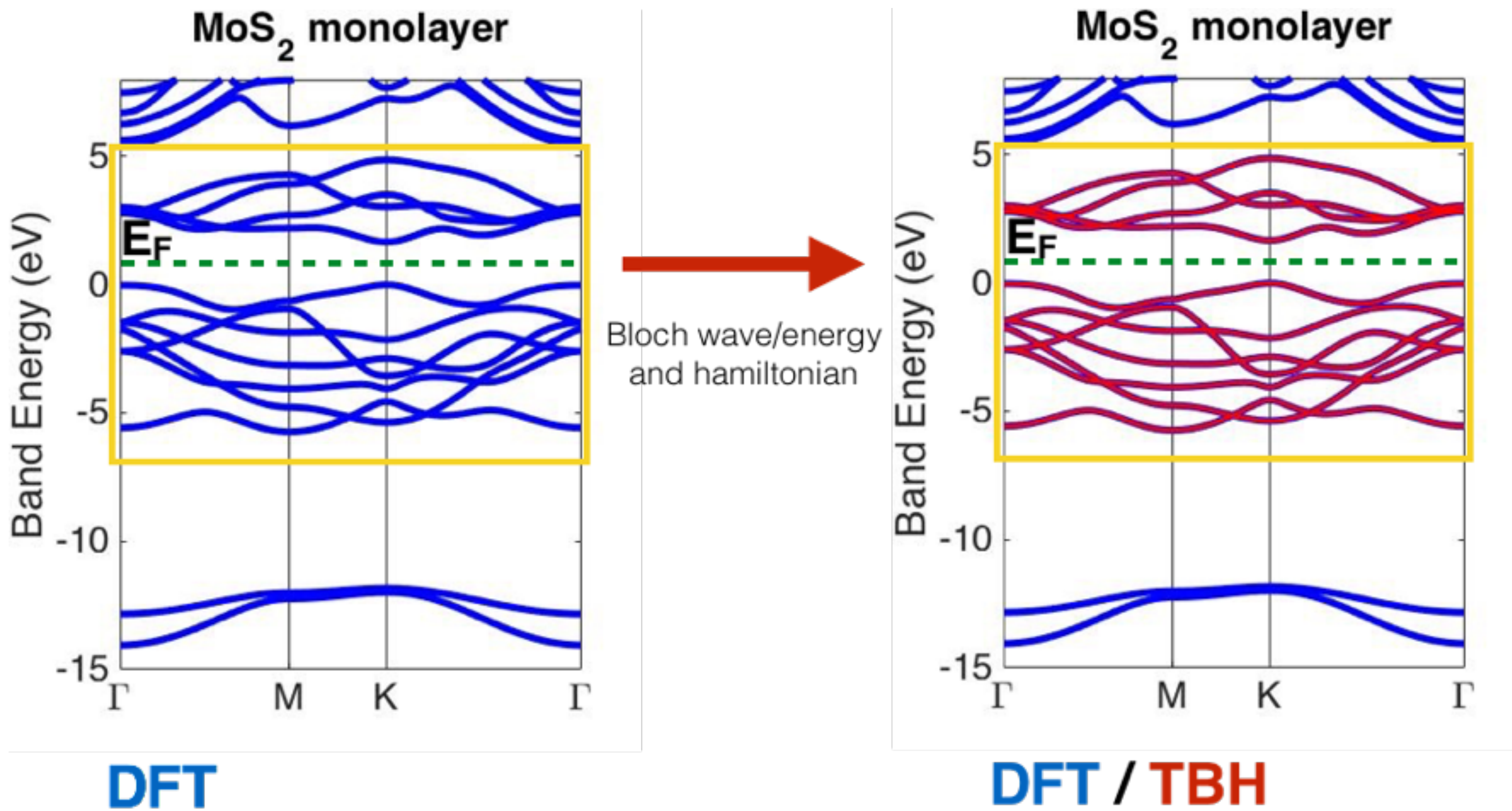
Wannier Functions: Localized Basis



$$|w_n(\vec{R})> = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}}[\sum_m U_{mn}^{(\vec{k})}|\psi_m(\vec{k})>]e^{-i\vec{k}\vec{R}}dk$$

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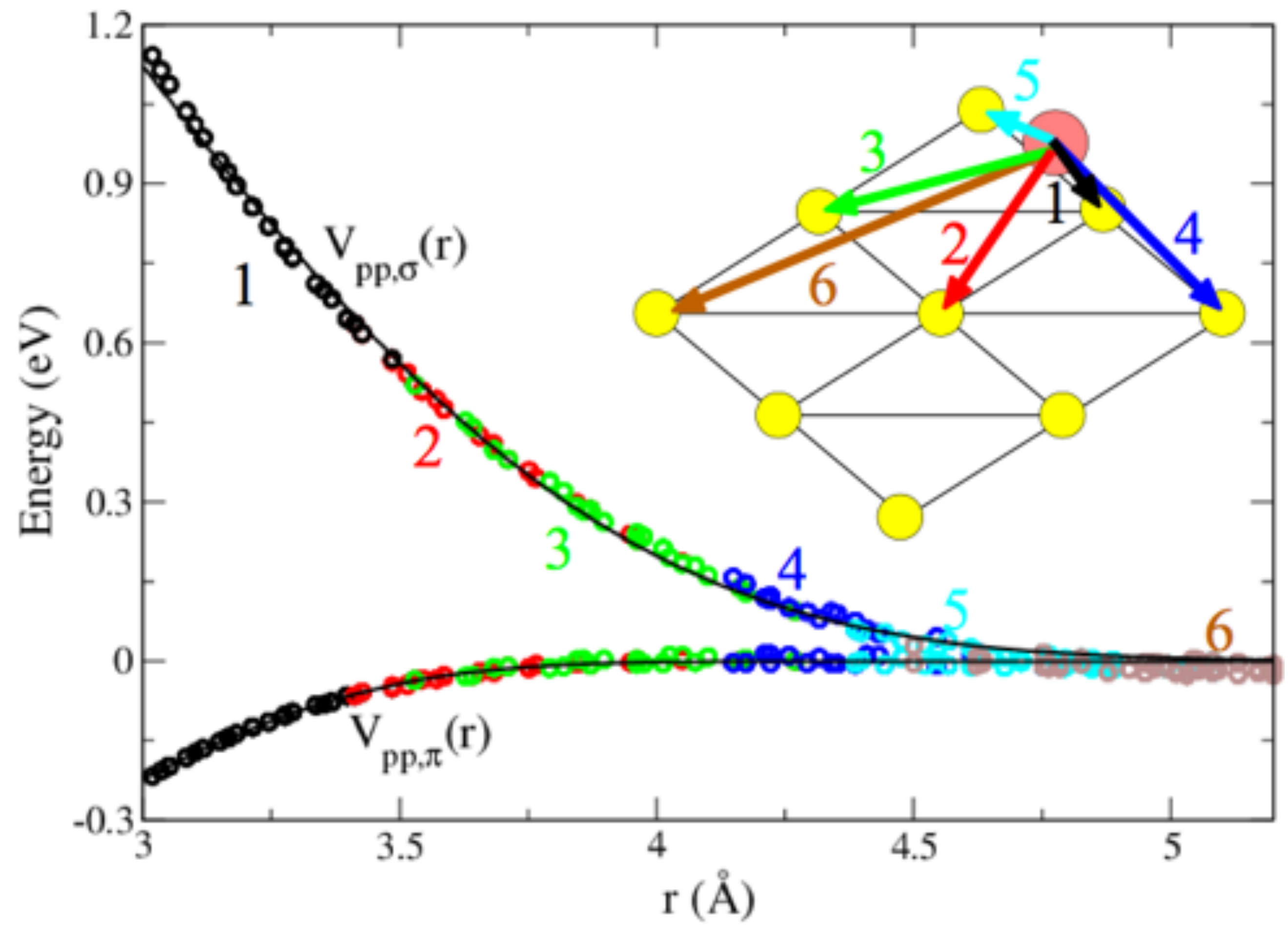
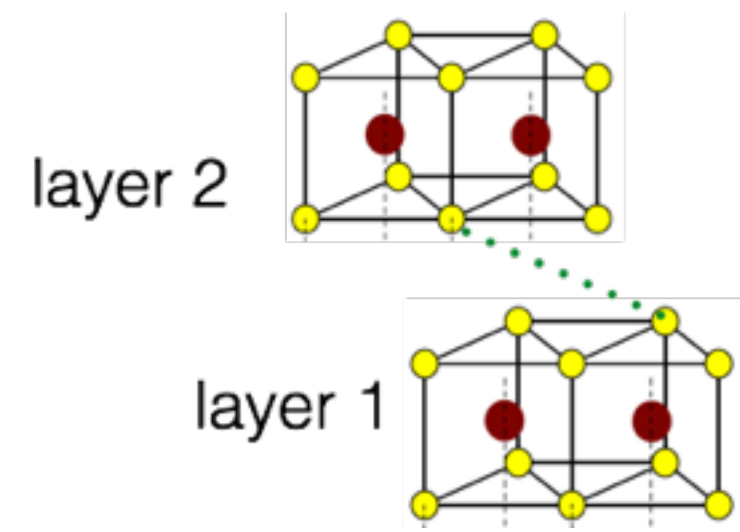
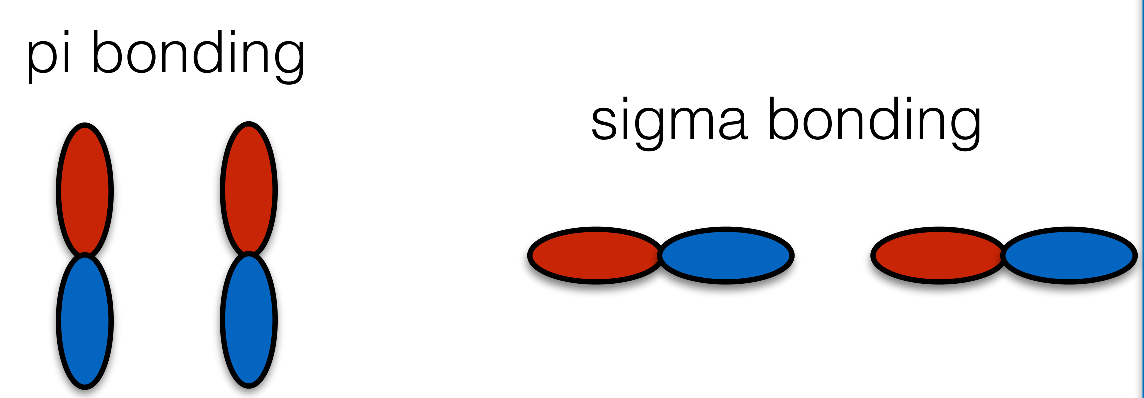
TMDC Interlayer Coupling



$$V_{pp,b}(r) = \nu_b \exp(-(r/R_b)^{\lambda_b})$$





two-center Slater-Koster approximation

Ref: Shiang Fang et al., Phys. Rev. B 92, 205108 (2015)

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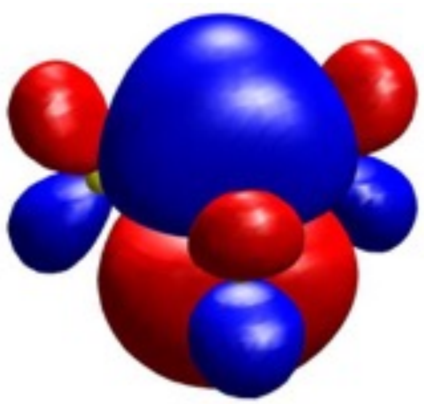
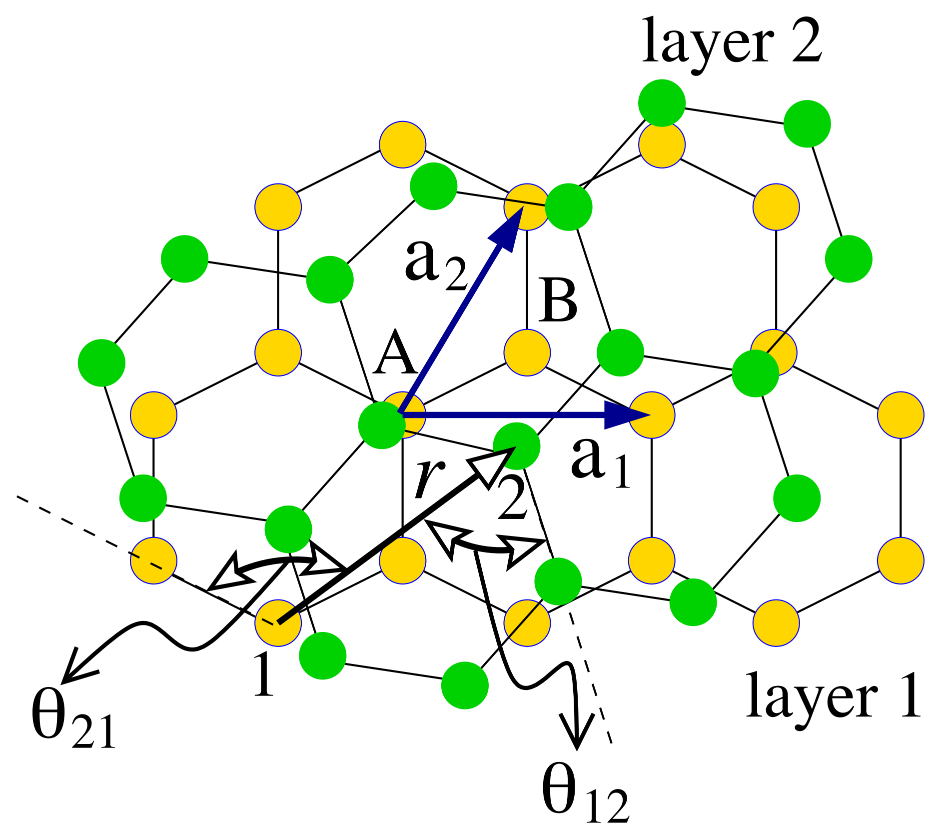
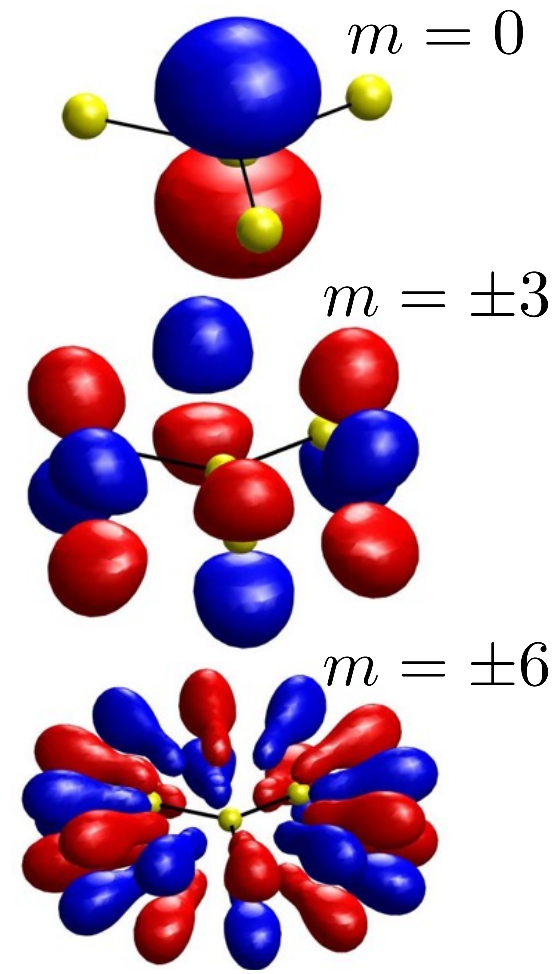
Graphene Interlayer Coupling

Pz Wannier function





Wannier function decomposition



$$t(\vec{r}) = V_0(r) + V_3(r)[\cos(3\theta_{12}) + \cos(3\theta_{21})] + V_6(r)[\cos(6\theta_{12}) + \cos(6\theta_{21})]$$

Ref: Shiang Fang et al., Phys. Rev. B 93, 235153 (2016)

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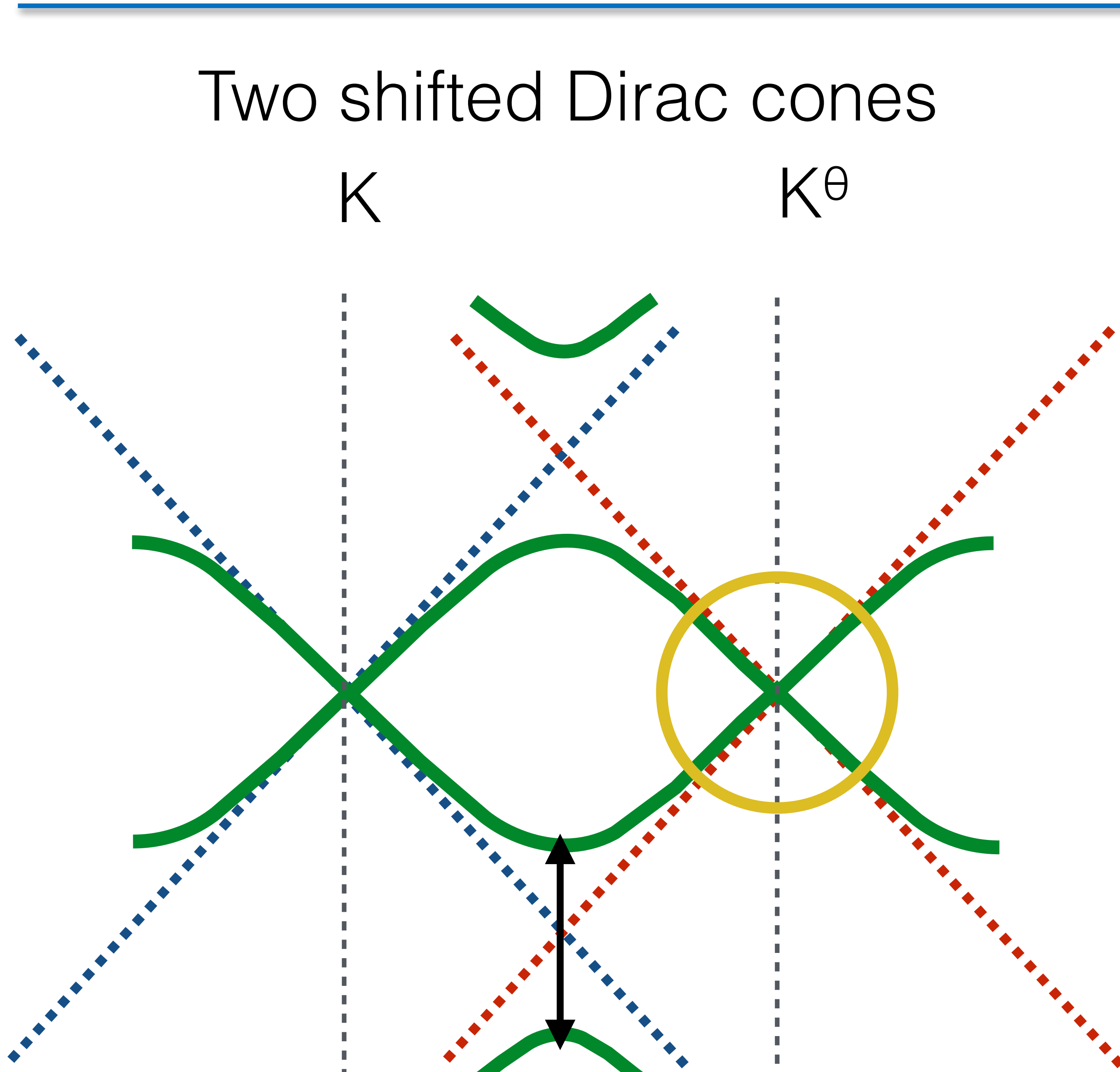
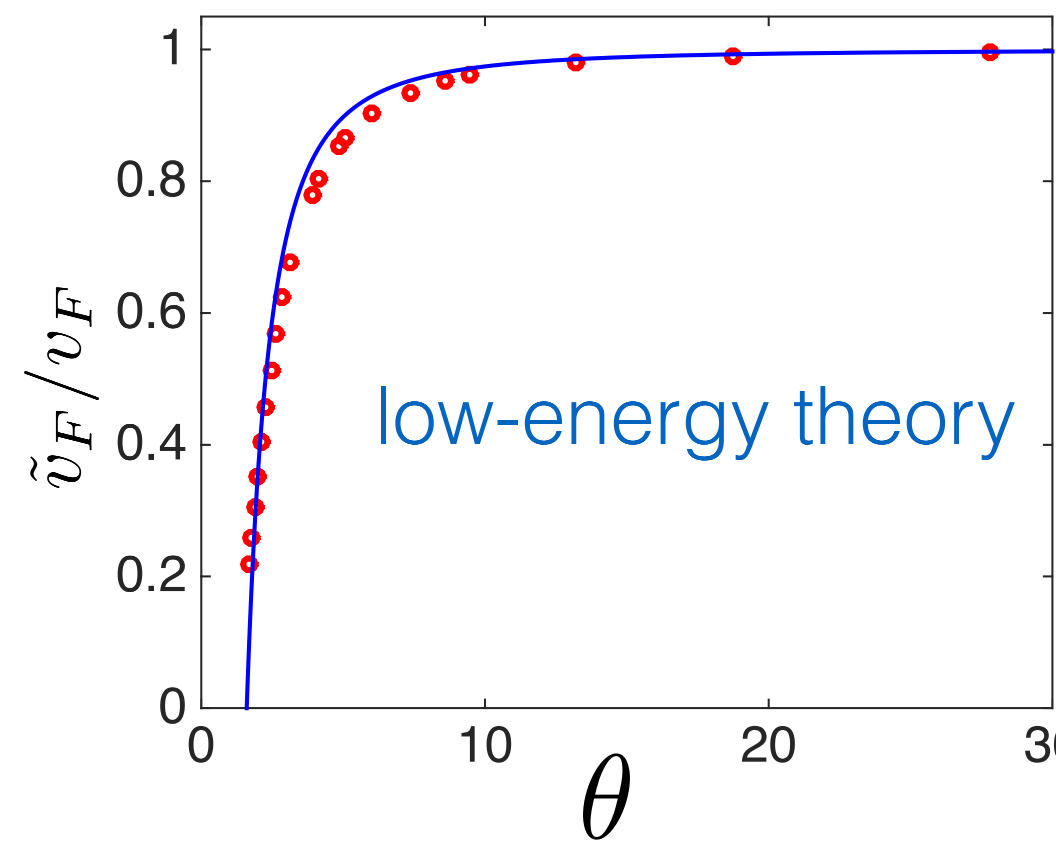
Graphene bilayer with a twist

Two shifted Dirac cones



Renormalization of Fermi velocity (slope near K)



$$\tilde{v}_F/v_F = 1 - C/\sin^2(\theta/2)$$

C ~ $2\text{x}10^{-4}$, vanishes at ~1.6

Ref: J. M. B. Lopes dos Santos et al., PRL 99, 256802 (2007)

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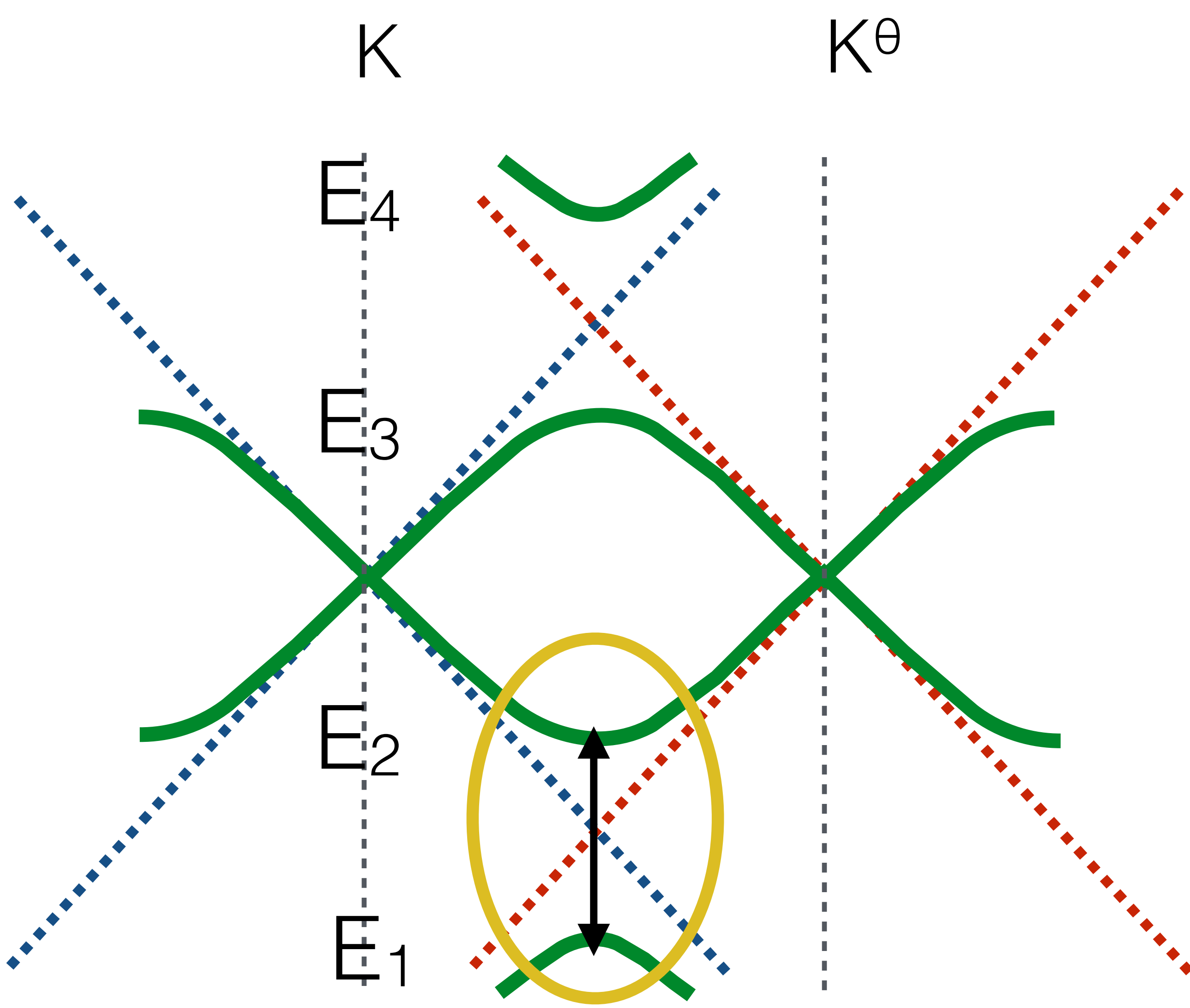
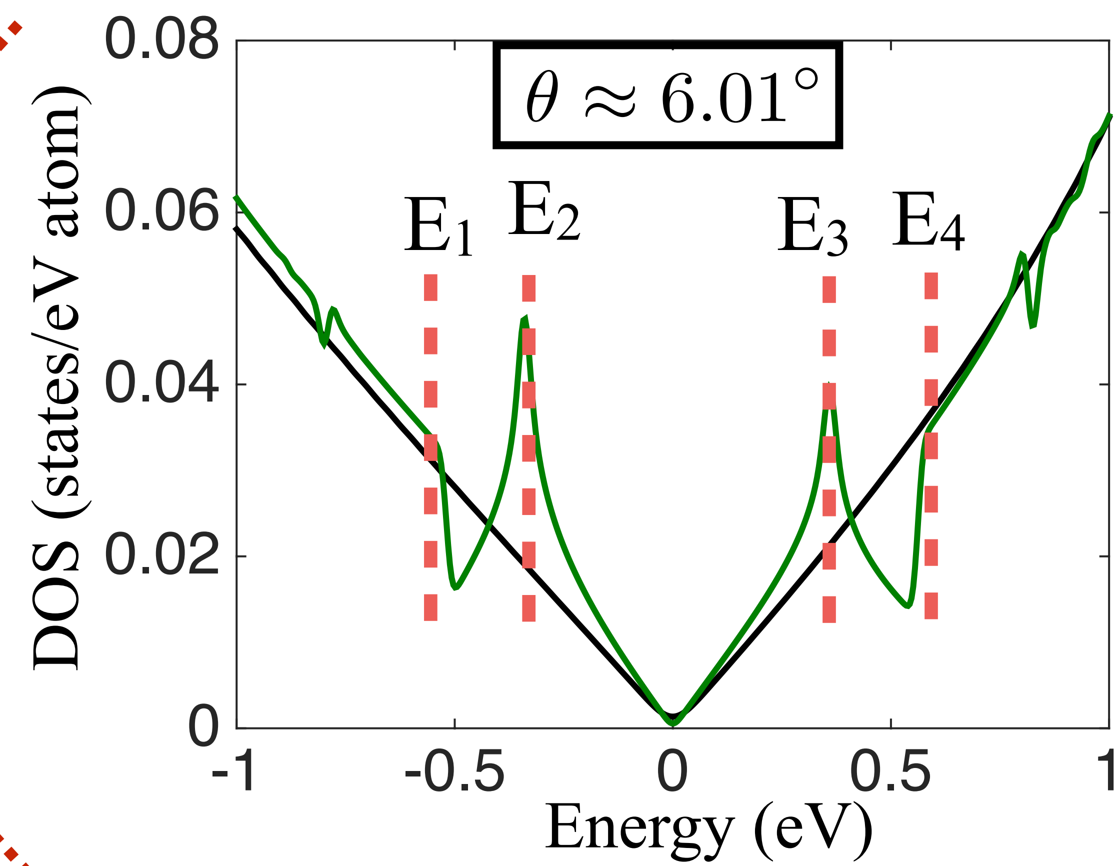


Van Hove singularity in density of states



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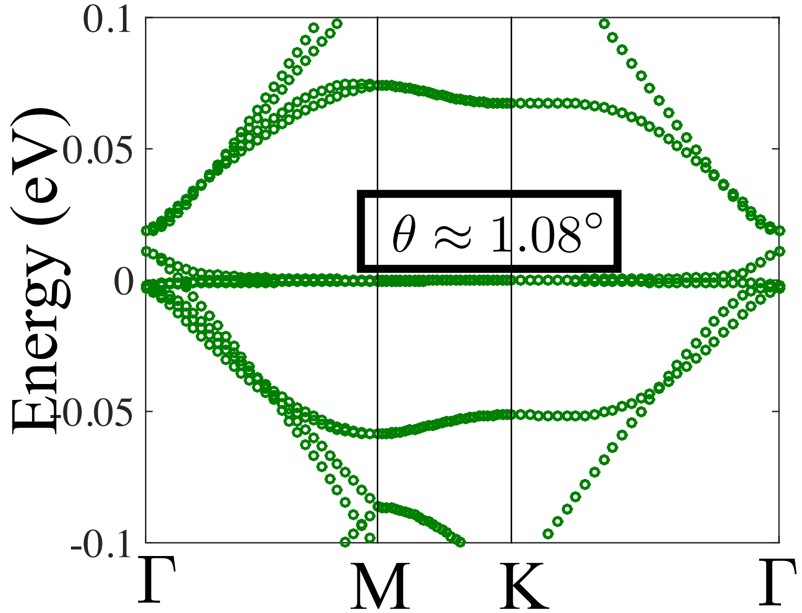
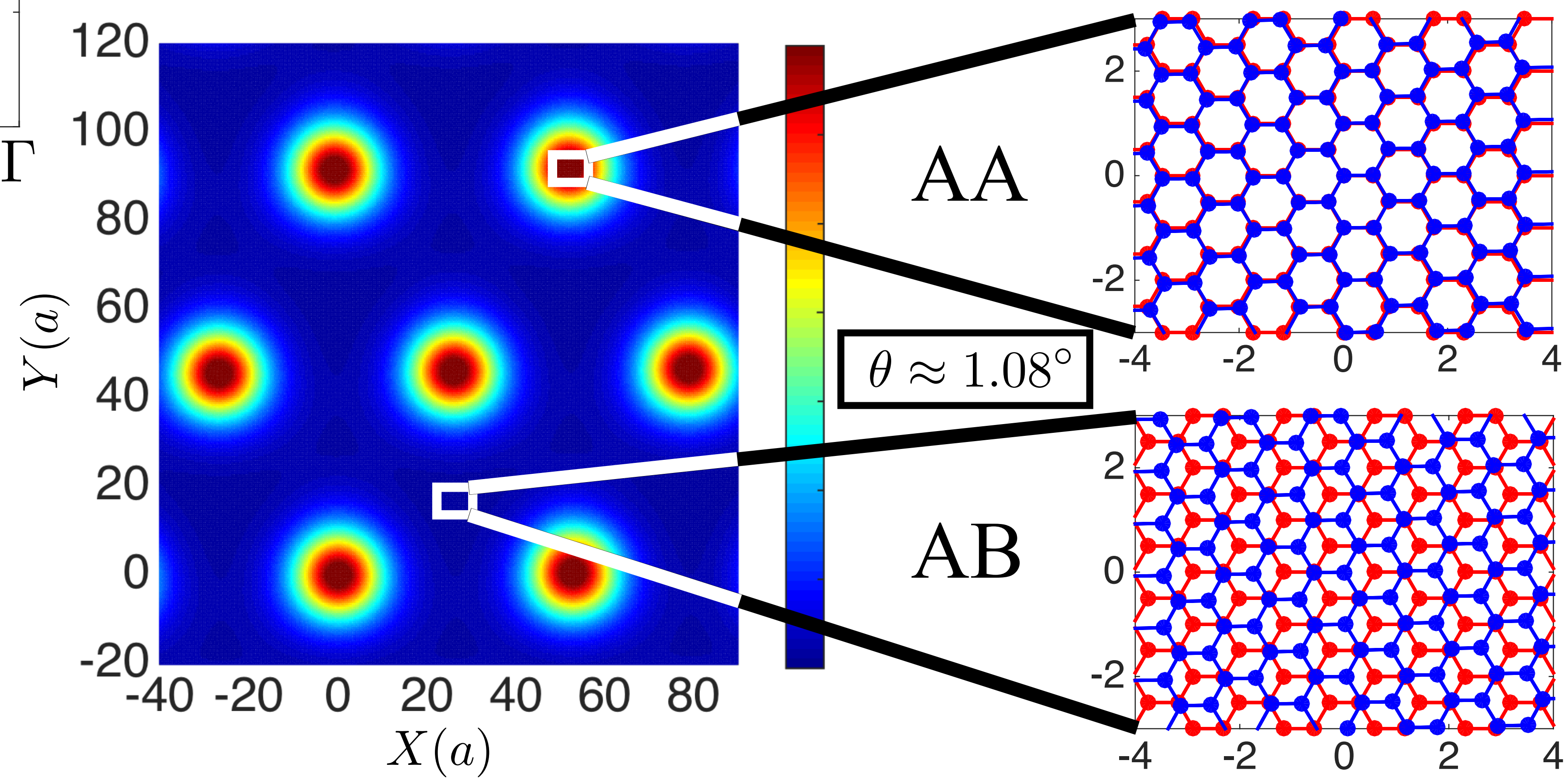
Flat Bands and Moiré Pattern



(31,30) twist structure (N=11164) with angle ~ 1°, we observe:

- The flat bands through out the whole BZ.

- Moiré pattern: charge distribution for the flat bands: highly localized at AA-sites



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Wannier and Topological Classification

"Ten-Fold Way" for topological classifications

		TRS	PHS	SLS	$d=1$	$d=2$	$d=3$
Standard (Wigner-Dyson)	A (unitary)	0	0	0	-	$\mathbb{Z}$	-
	AI (orthogonal)	+1	0	0	-	-	-
	AII (symplectic)	−1	0	0	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$
Chiral (sublattice)	AIII (chiral unitary)	0	0	1	$\mathbb{Z}$	-	$\mathbb{Z}$
	BDI (chiral orthogonal)	+1	+1	1	$\mathbb{Z}$	-	-
	CII (chiral symplectic)	−1	−1	1	$\mathbb{Z}$	-	$\mathbb{Z}_2$
BdG	D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	-
	C	0	−1	0	-	$\mathbb{Z}$	-
	DIII	−1	+1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	CI	+1	−1	1	-	-	$\mathbb{Z}$

Integer Quantum Hall; Chern insulator

Z2 Topological Insulator

Topological superconductivity / Majorana fermions

- Depending on the symmetry, there are different topological classes for the filled Hilbert space of a Hamiltonian.
- Non-zero Chern number gives obstructions for the construction of Wannier functions

Ref: Andreas P. Schnyder et al., Phys. Rev. B 78, 195125 (2008)

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Summary

- Ab-initio tight-binding hamiltonian from Wannier transformation based on density functional theory calculations as an efficient way of modeling the materials
- Specific examples with 2D layered heterostructure and the interlayer coupling models for graphene and TMDCs
- Wannier construction and the topological obstructions in the presence of non-zero Chern numbers

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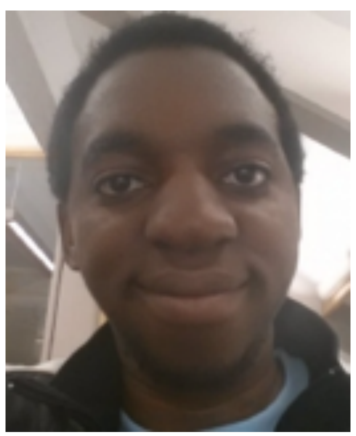

Rodrick Kate Defo

Sharmila Shirodkar

Tuesday 19:30-20:15 poster session with Stephen
Thursday 9:45-10:45 (Daniel, Stephen and Paul), applications based on Wannier tight-binding models for especially large scale incommensurate 2D layered heterostructure simulations

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