A band-free approach to twistronics

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Workshop on Theory and Computation for 2D Materials

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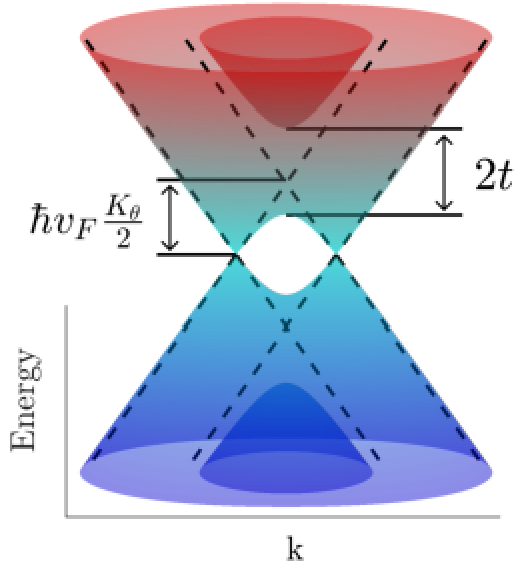
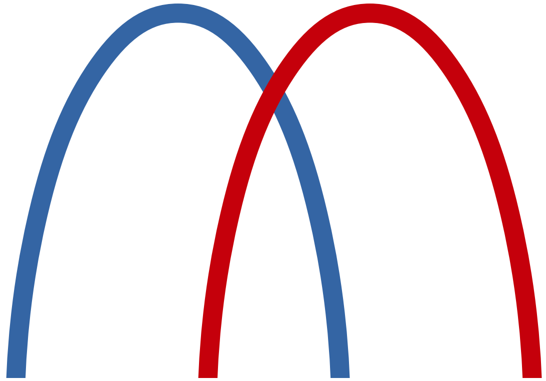
Modeling moiré systems

Semimetals:



Semiconductors:



Modeling moiré systems

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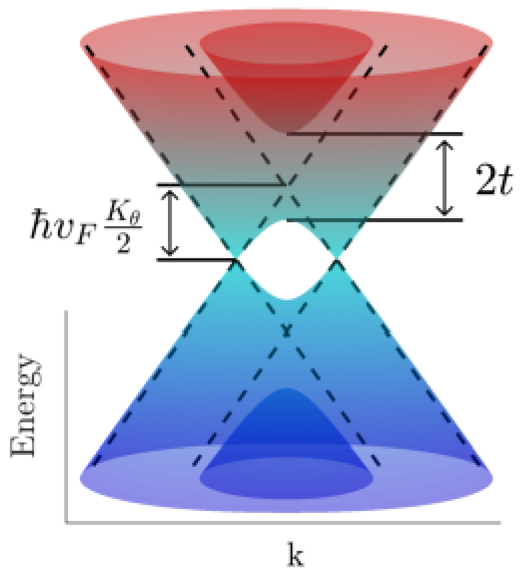

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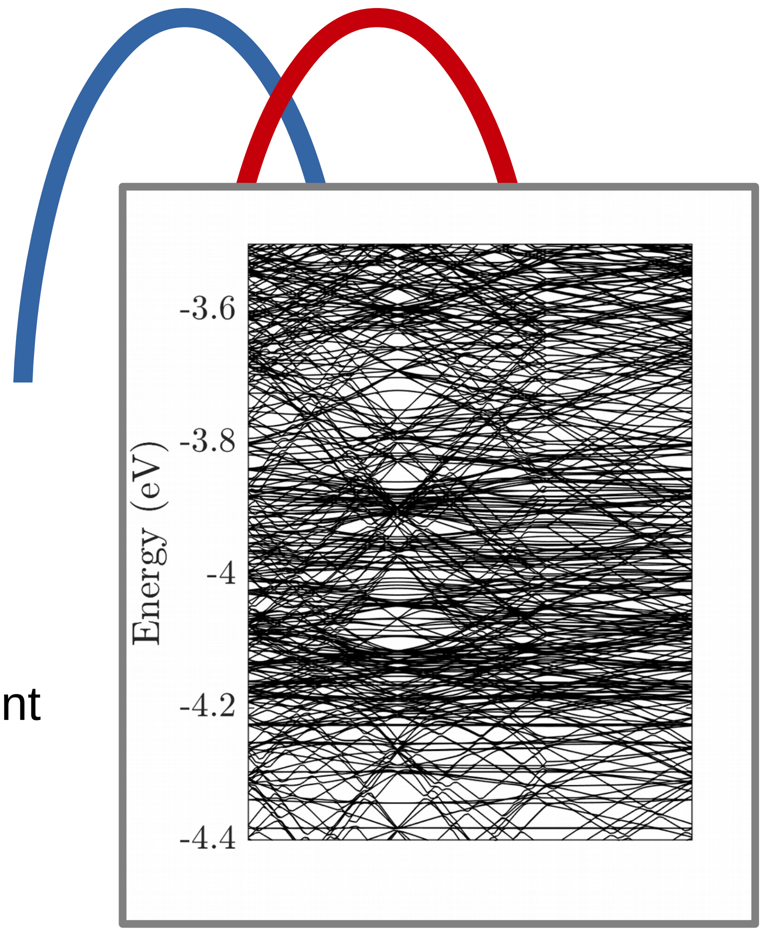


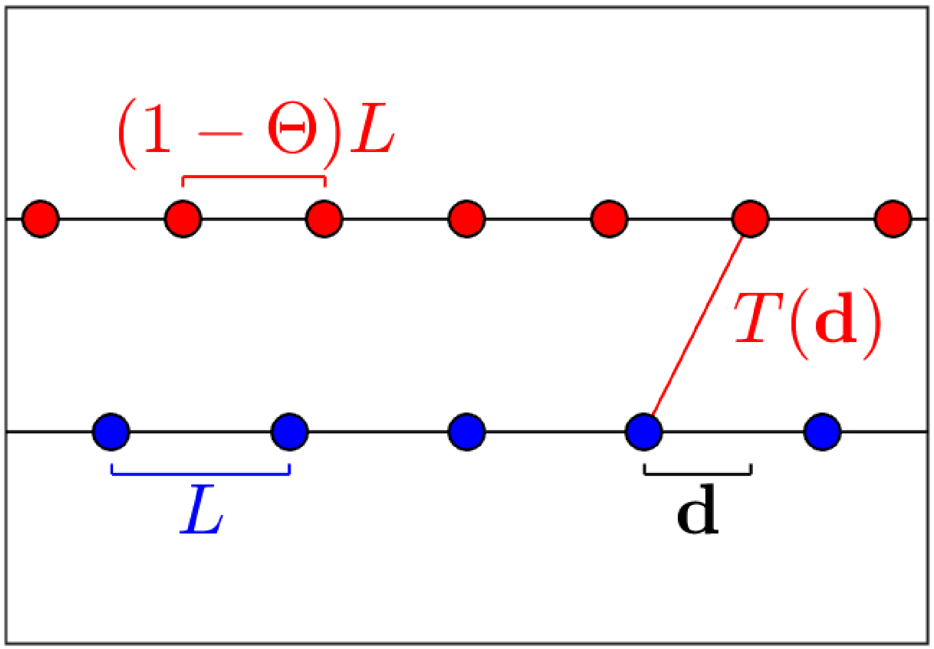
Problem: Materials with multiple bands, metallic regions

Goal: Predict twistronic effects in any spectral environment

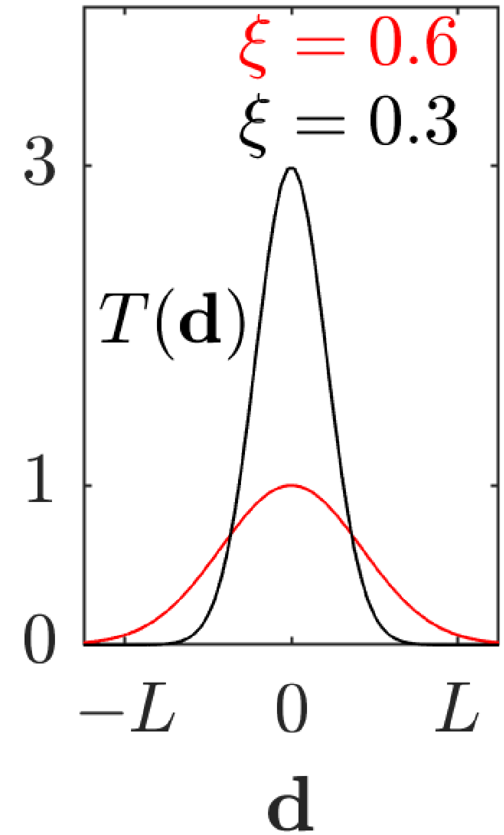
How: Look at stacking-dependent local density of states

1D moire model

Side view



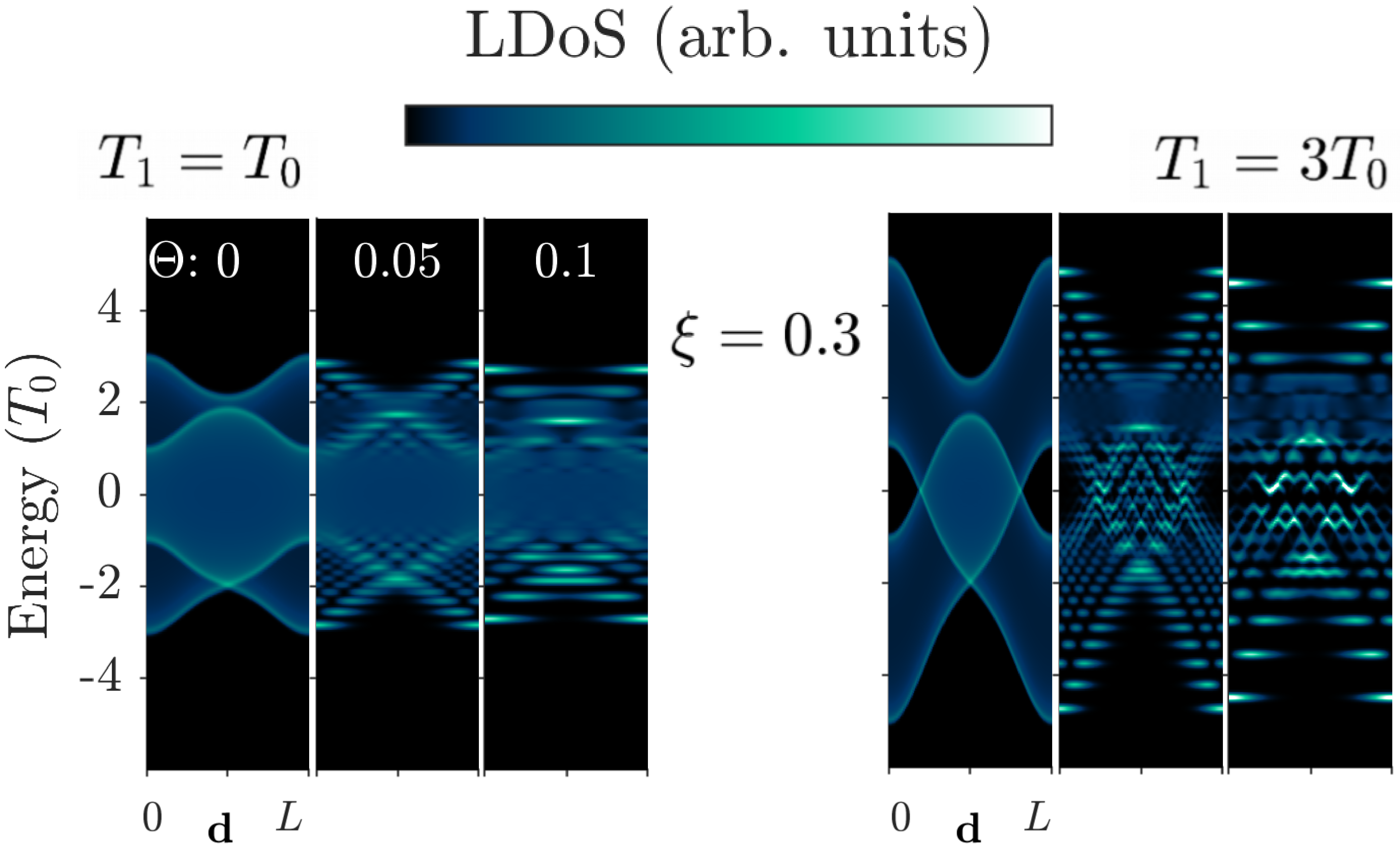
Interlayer coupling



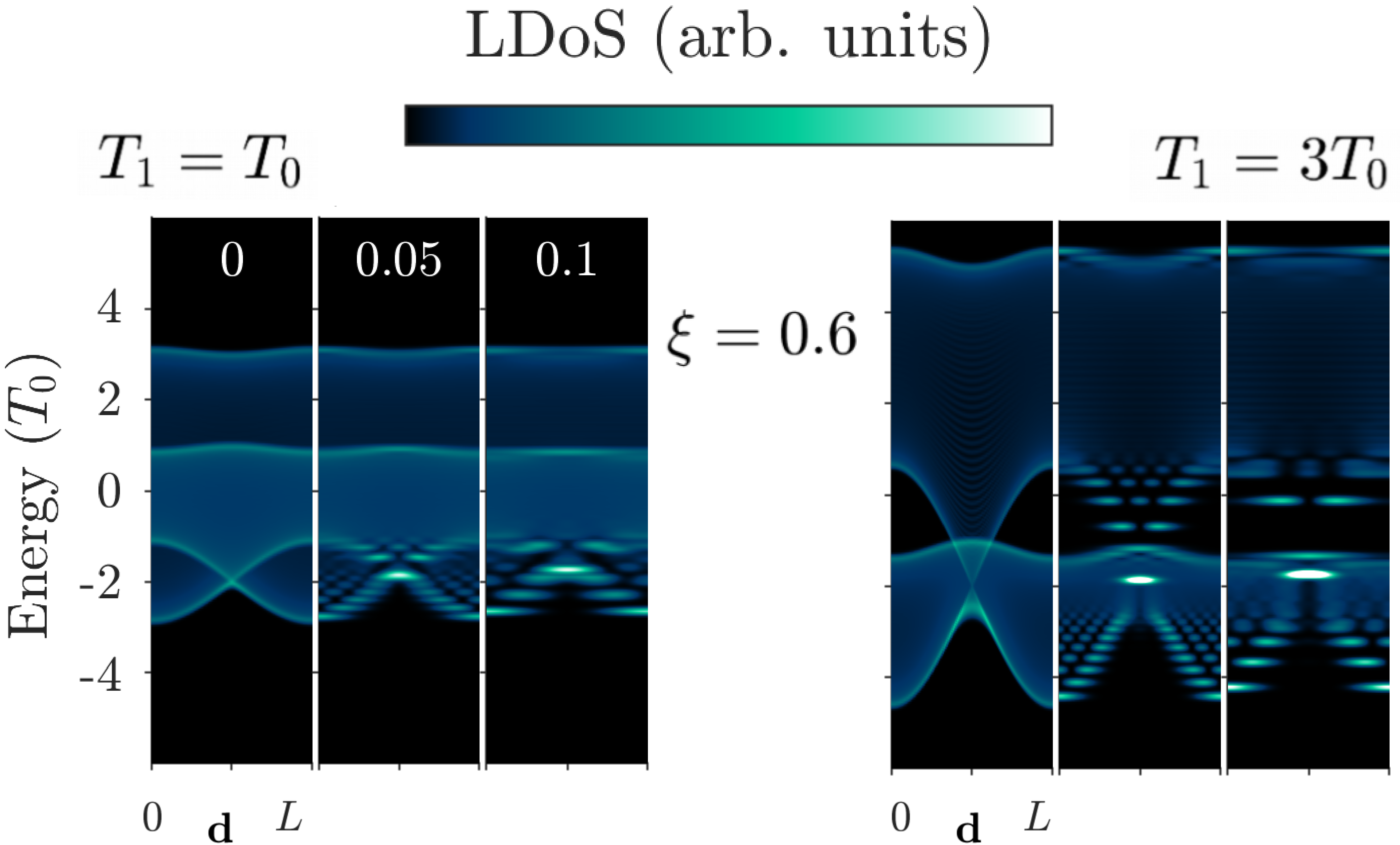
Uniform moiré in 2D: 3 Choices
    Rotation, Lattice mismatch, Shear

Uniform moiré in 1D: 1 Choice
    Lattice mismatch

$$T(\mathbf{d}) = T_1 e^{-(d/\xi)^2}$$



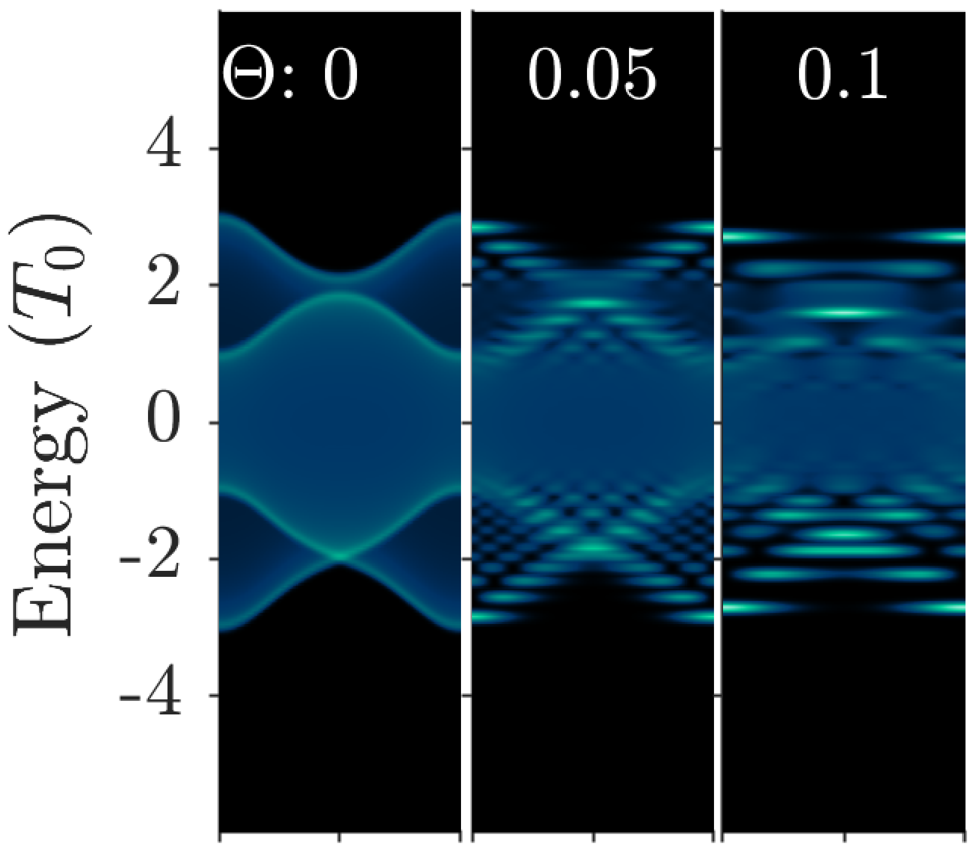
LDoS (arb. units)
$T_1 = T_0$
$T_1 = 3T_0$
Θ: 0
0.05
0.1
$\xi = 0.3$
Energy (T_0)
4
2
0
-2
-4
0
d
L
0
d
L



Increased interlayer coupling range:

- Stronger average coupling
- Weaker variation

Harmonic oscillator flat bands



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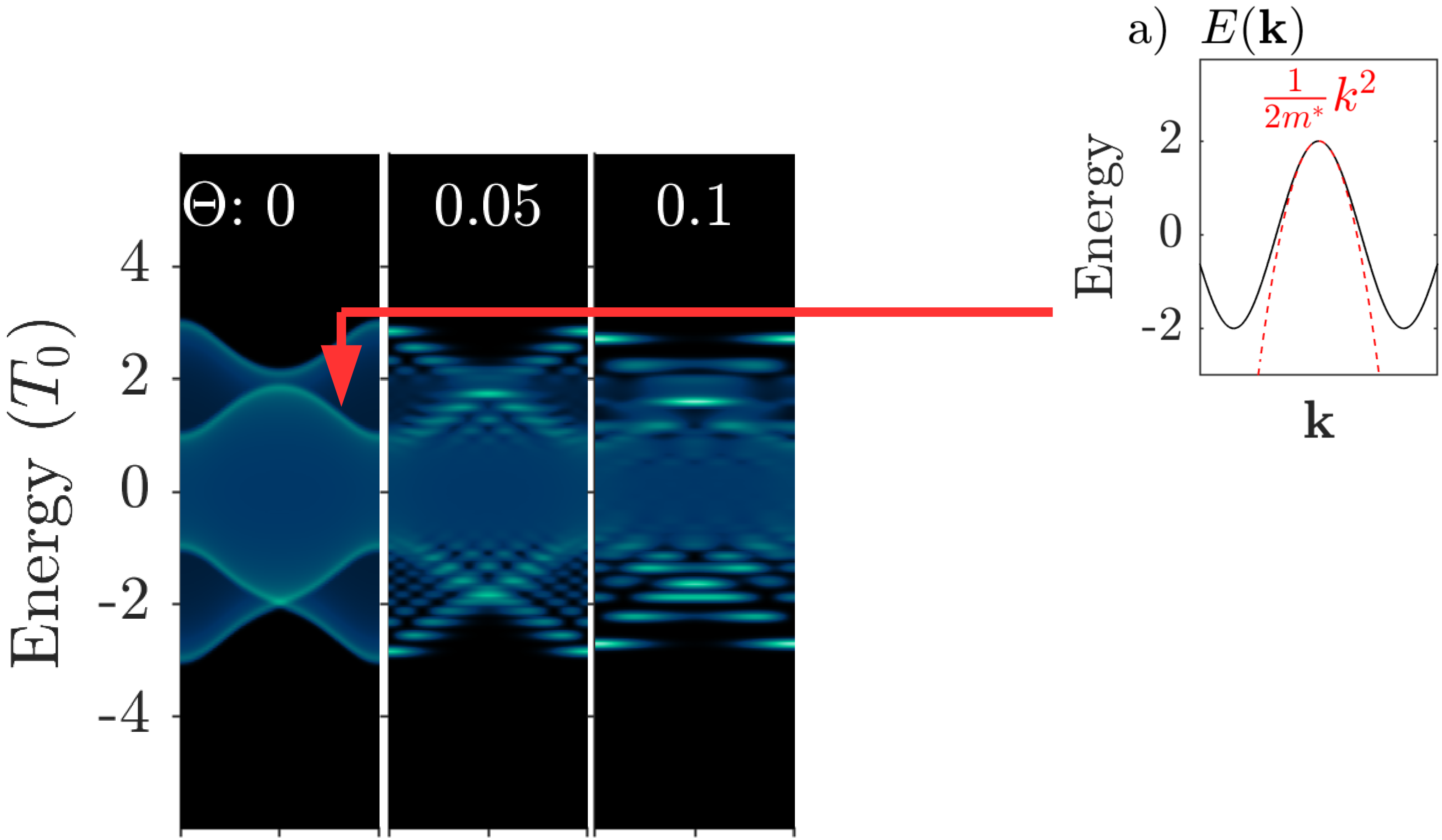

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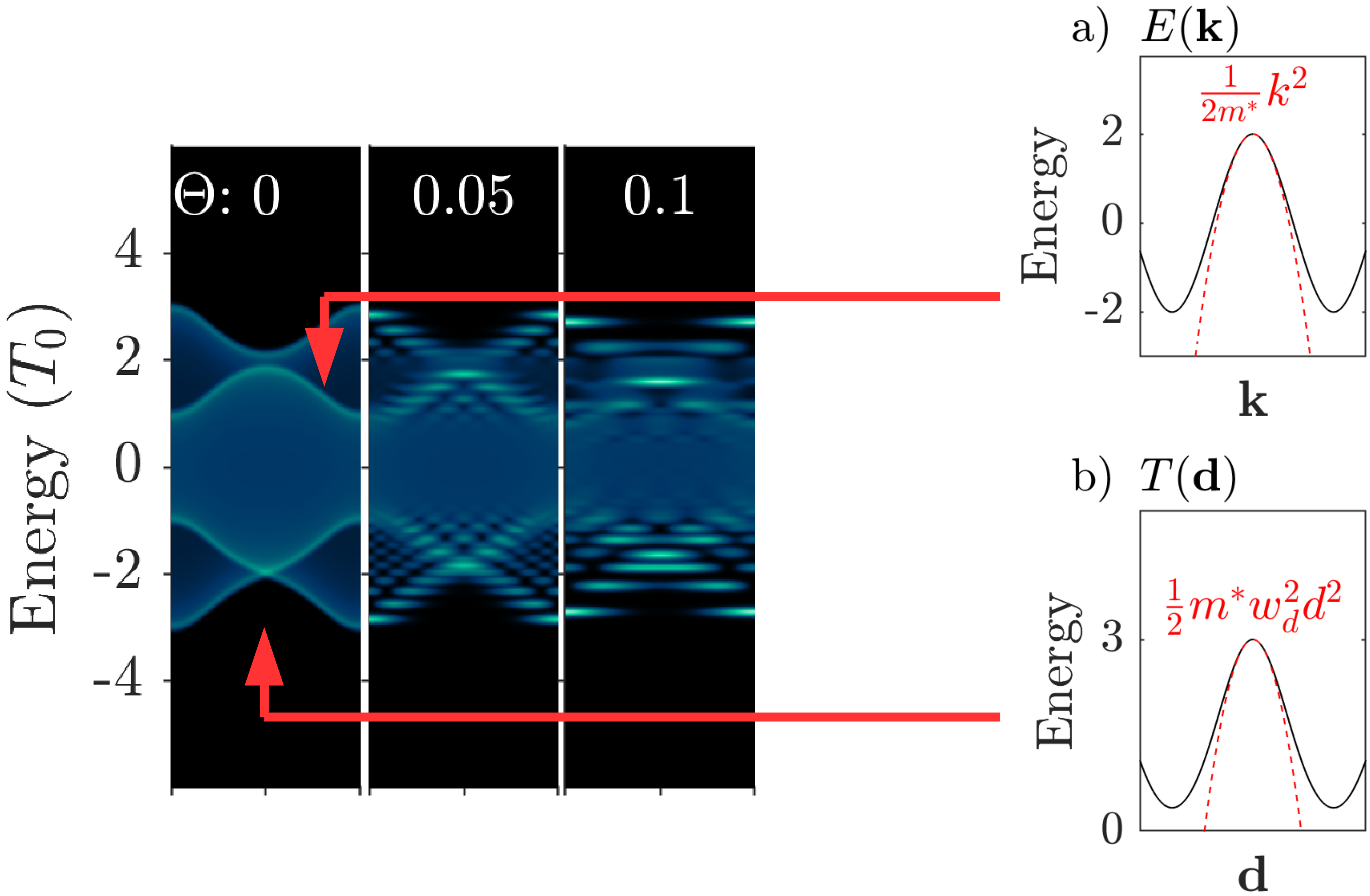

Harmonic oscillator flat bands

$$H = \frac{1}{2m^*}(\psi_1^\dagger \partial^2 \psi_1 + \psi_2^\dagger \partial^2 \psi_2) + T_{12}(\boldsymbol{r})(\psi_1^\dagger \psi_2 + h.c.).$$

Harmonic oscillator flat bands

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$$\boxed{\psi_\pm = \frac{1}{\sqrt{2}}\left(\psi_1 \pm \psi_2\right)}$$

$$H_\pm = \frac{1}{2m^*}(\psi_\pm^\dagger \partial^2 \psi_\pm) \pm T_{12}(\boldsymbol{r})\psi_\pm^\dagger \psi_\pm.$$

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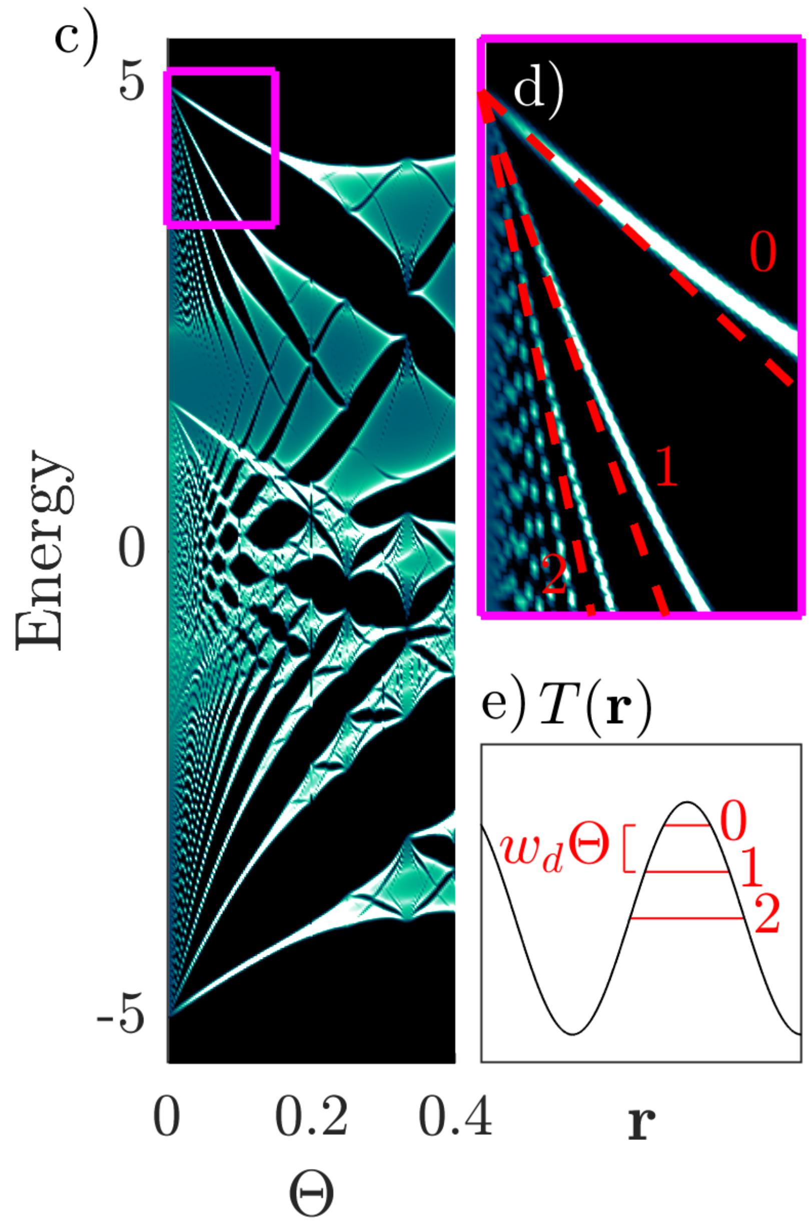
$$H_\pm = \psi_\pm^\dagger \left(\frac{1}{2m^*} \partial^2 \pm \frac{1}{2} m^* \omega^2 r^2 \right) \psi_\pm.$$

$$\boxed{\omega = \pi \Theta L \sqrt{2 T_0 T_1} = \omega_\Theta \Theta}$$

Harmonic oscillator flat bands



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Unpacking the oscillator equation

$$H_{\pm} = \frac{1}{2m^*}(\psi_{\pm}^{\dagger}\partial^2\psi_{\pm}) \pm T_{12}(\boldsymbol{r})\psi_{\pm}^{\dagger}\psi_{\pm}.$$

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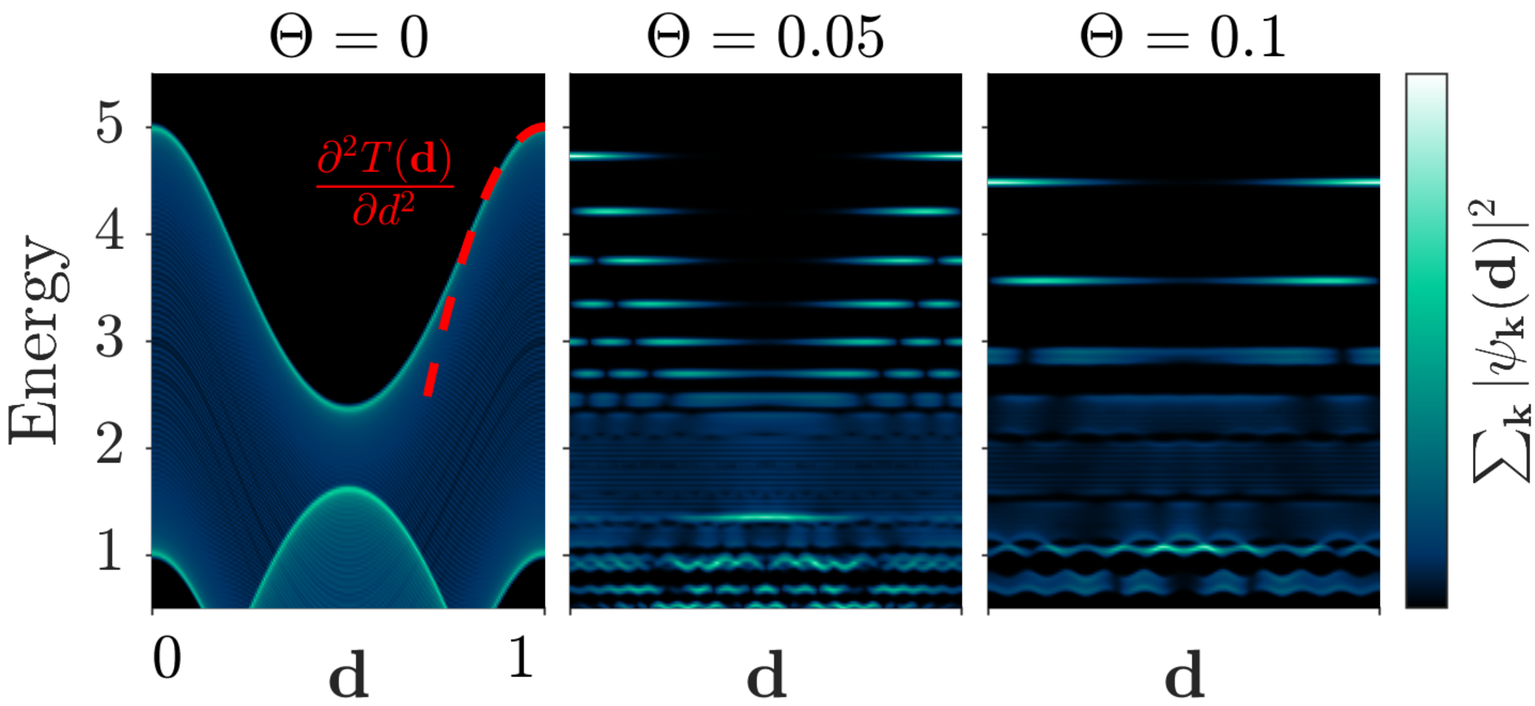
$$\omega = \omega_{\Theta}\Theta = \Theta\left(\frac{\partial^2 E(\mathbf{k})}{\partial \mathbf{k}^2}\right)\left(\frac{\partial^2 T(\mathbf{d})}{\partial \mathbf{d}^2}\right)$$

Unpacking the oscillator equation



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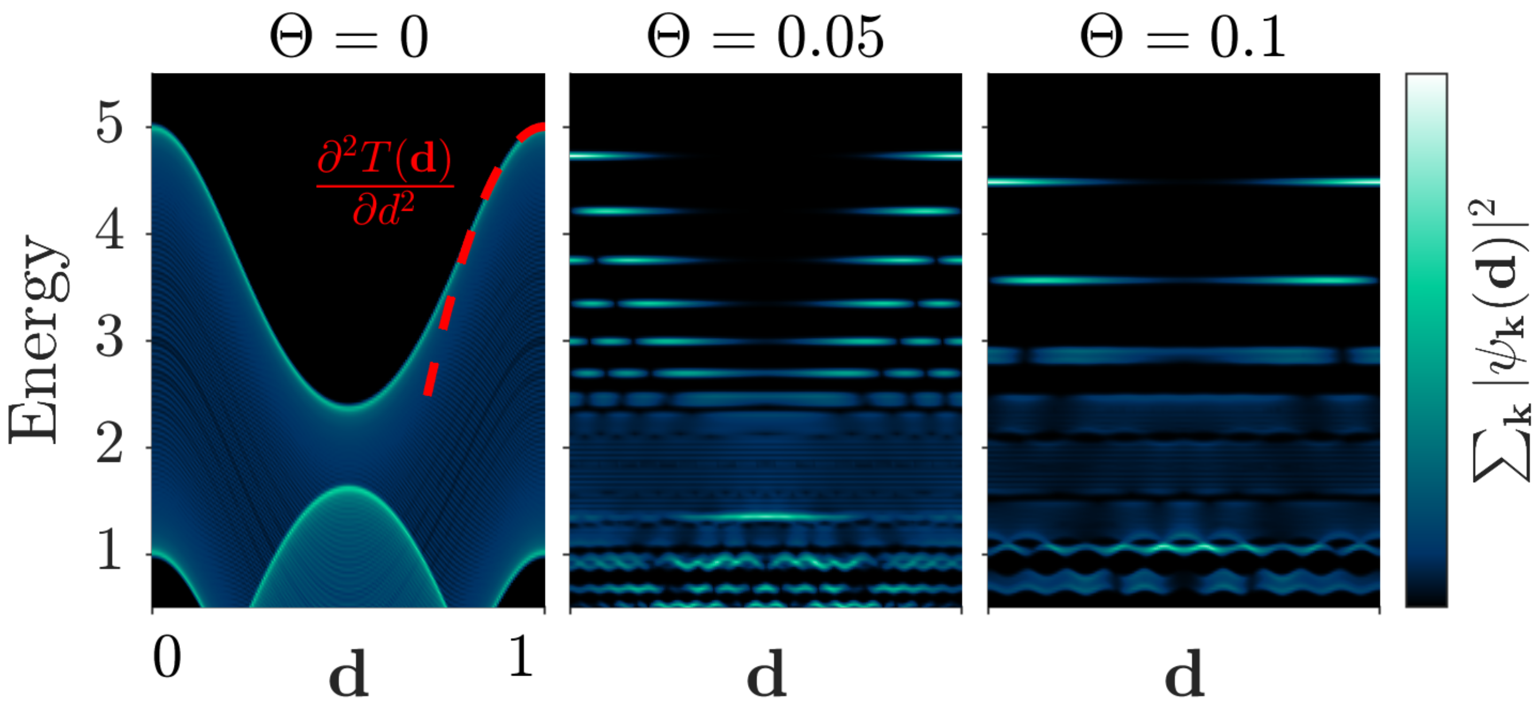

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Loss of confining well
→ No confined levels

Configuration-Momentum Duality

$$\mathrm{LDoS}(\mathbf{d}) = \sum_{\mathbf{k}} |\psi_{\mathbf{k}}(\mathbf{d})|^2$$

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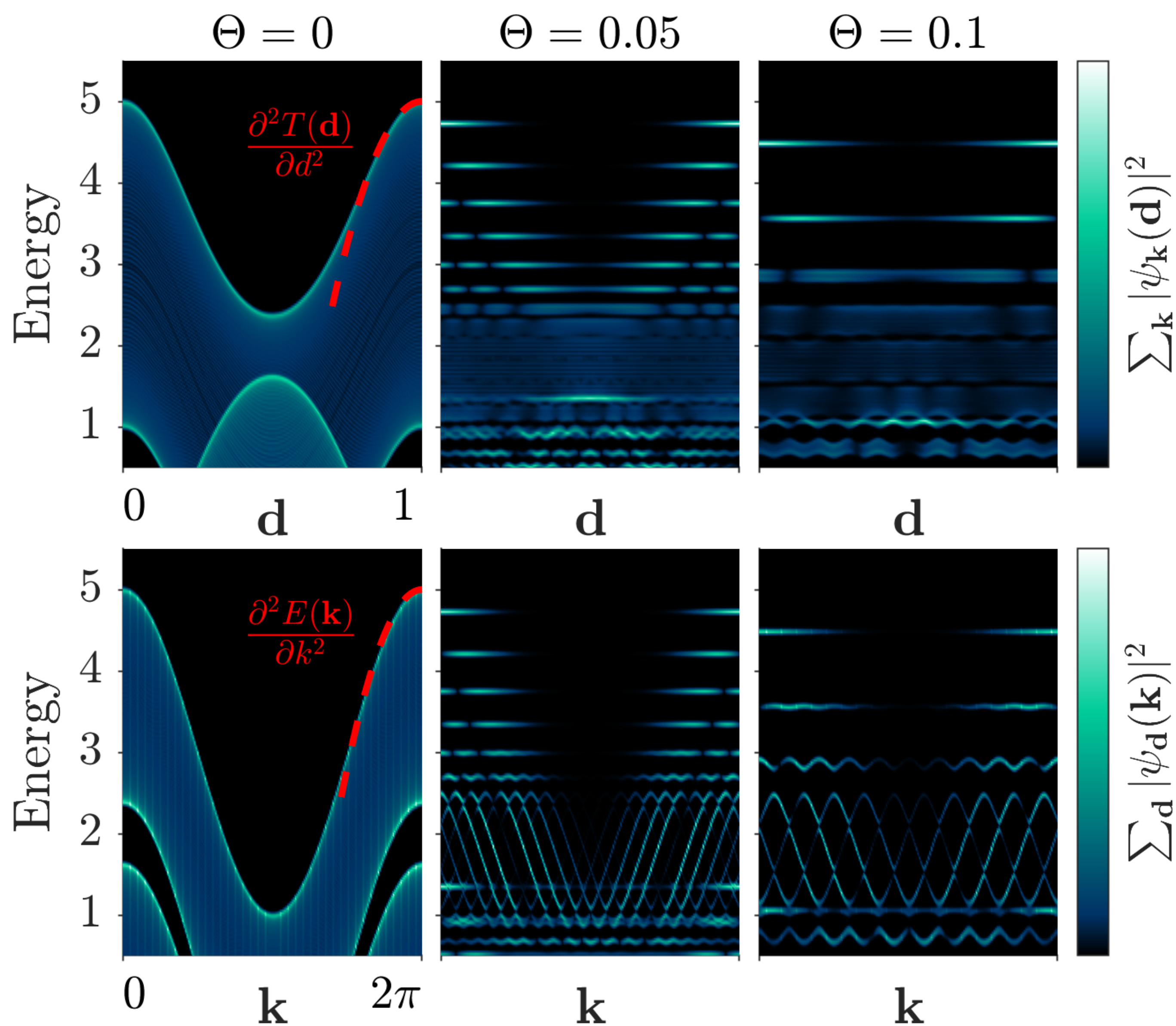
$$\Updownarrow$$

$$\mathrm{LDoS}(\mathbf{k}) = \sum_{\mathbf{d}} |\psi_{\mathbf{d}}(\mathbf{k})|^2$$

Momentum-projected local density of states,
averaged over all interlayer configurations

Configuration-Momentum Duality

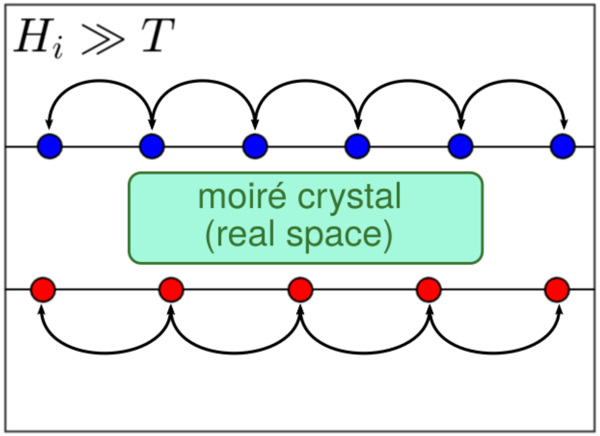


The other harmonic failure

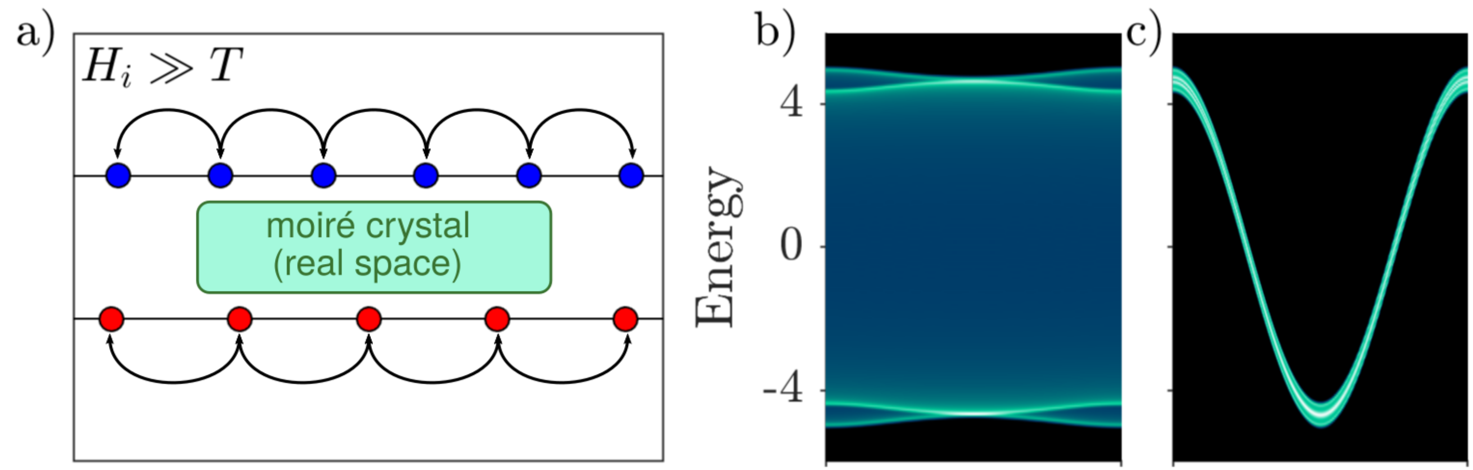
$$\omega = \omega_\Theta \Theta = \Theta \left(\frac{\partial^2 E(\mathbf{k})}{\partial \mathbf{k}^2} \right) \left(\frac{\partial^2 T(\mathbf{d})}{\partial \mathbf{d}^2} \right)$$

Two types of crystals

a)



Two types of crystals



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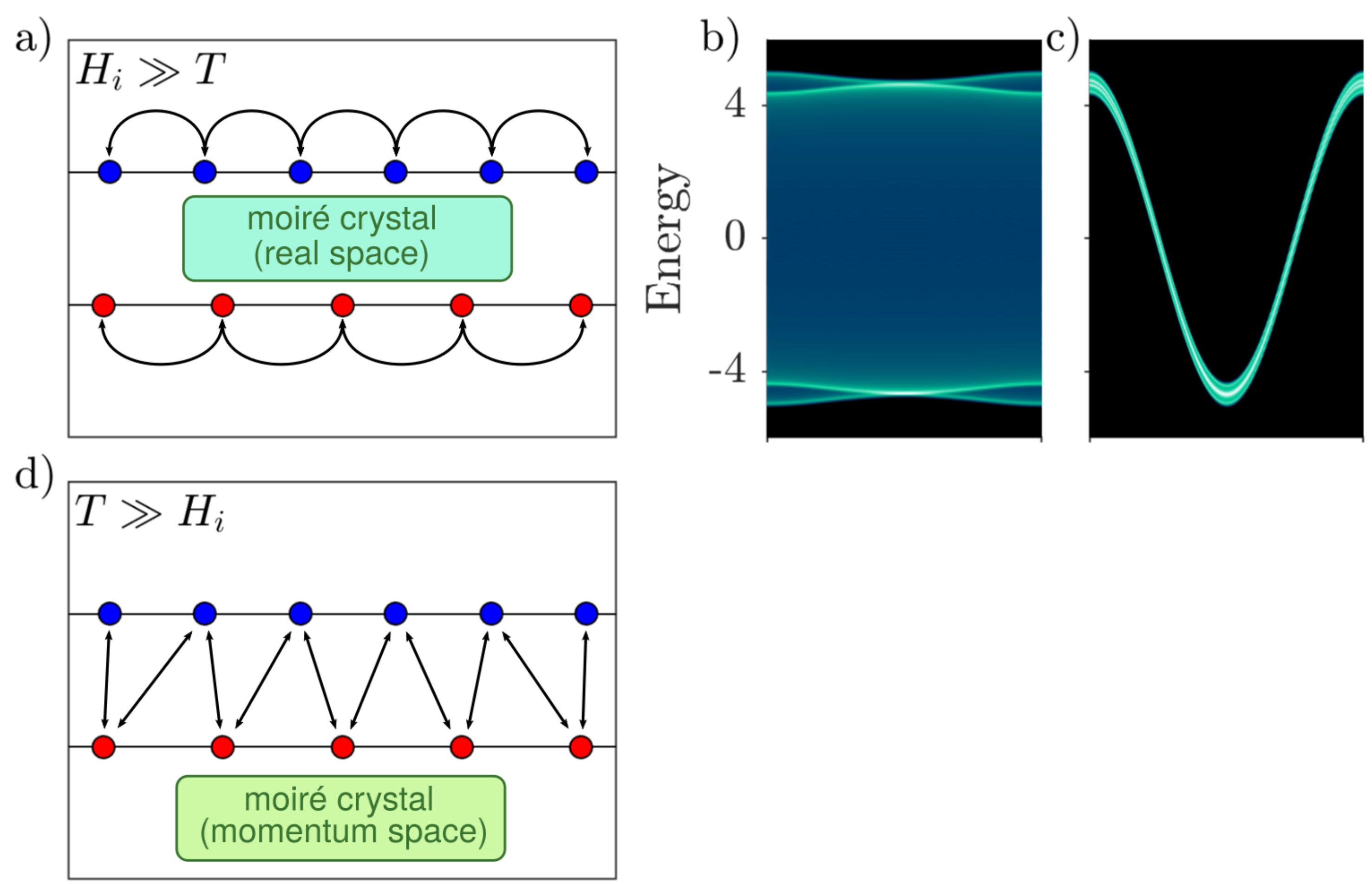

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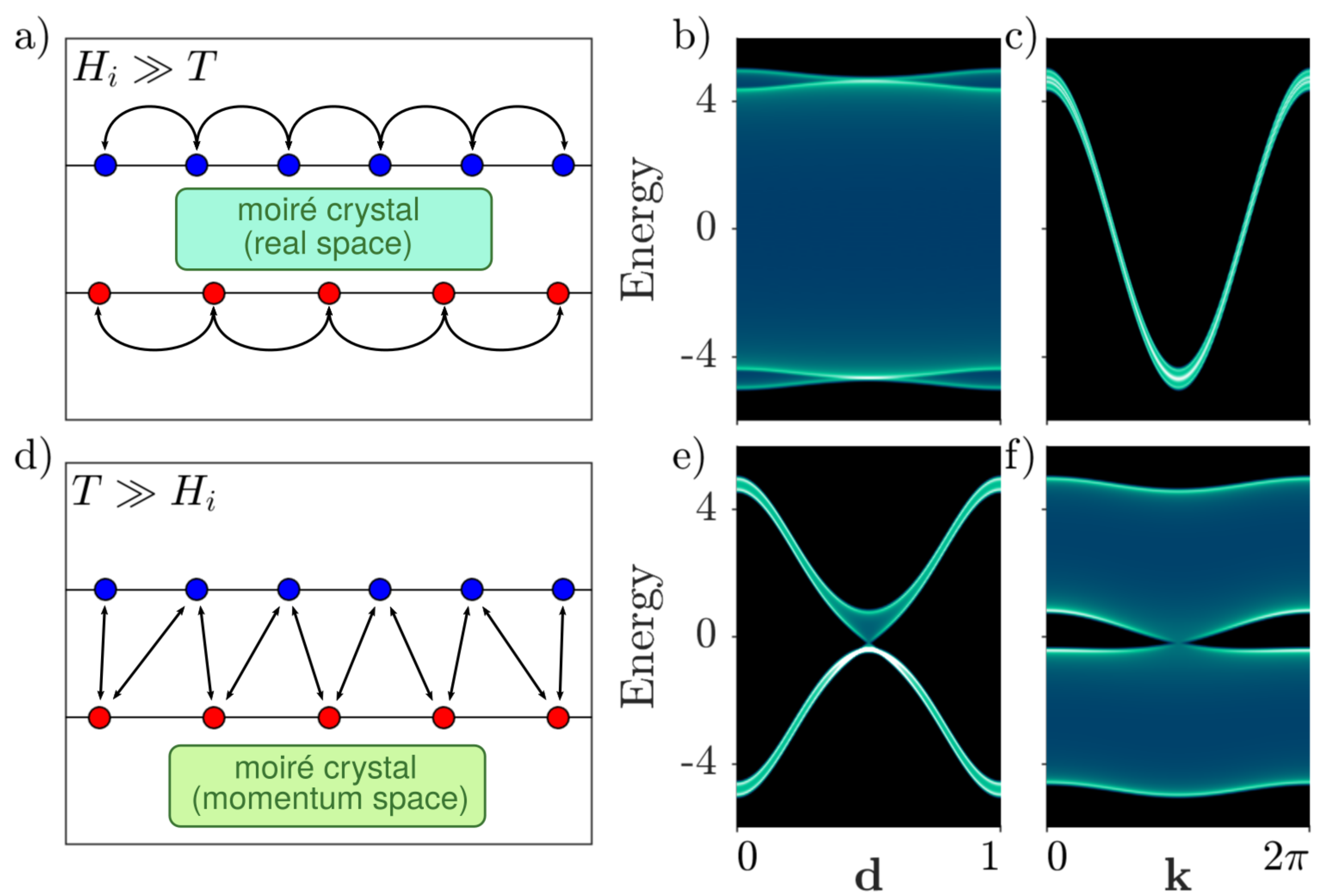
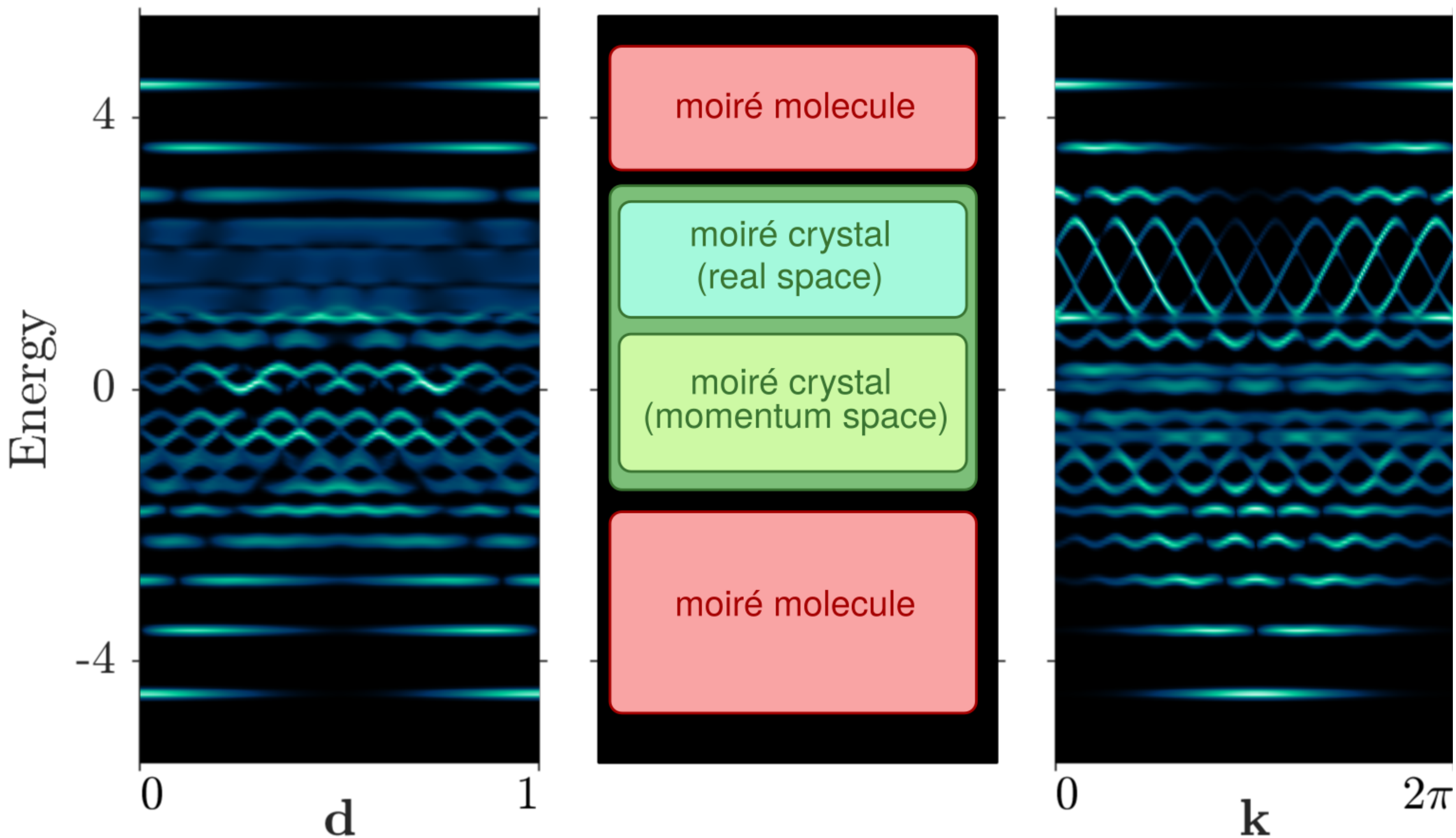
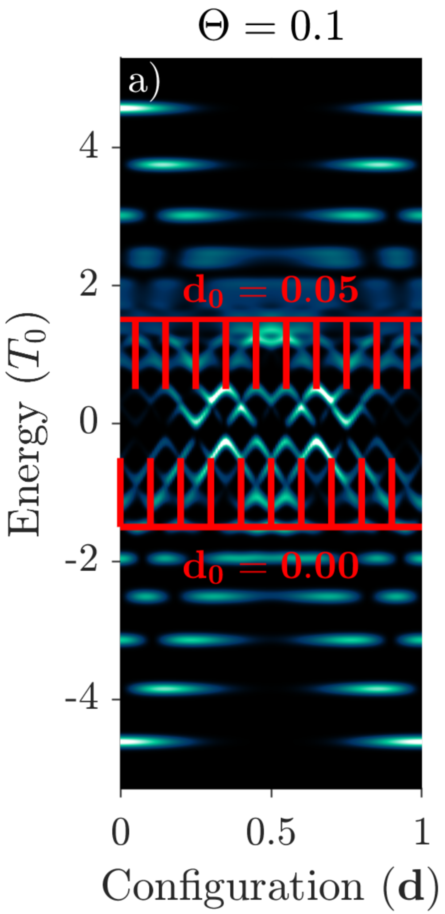


Twistronic classification



Momentum crystal in real-space



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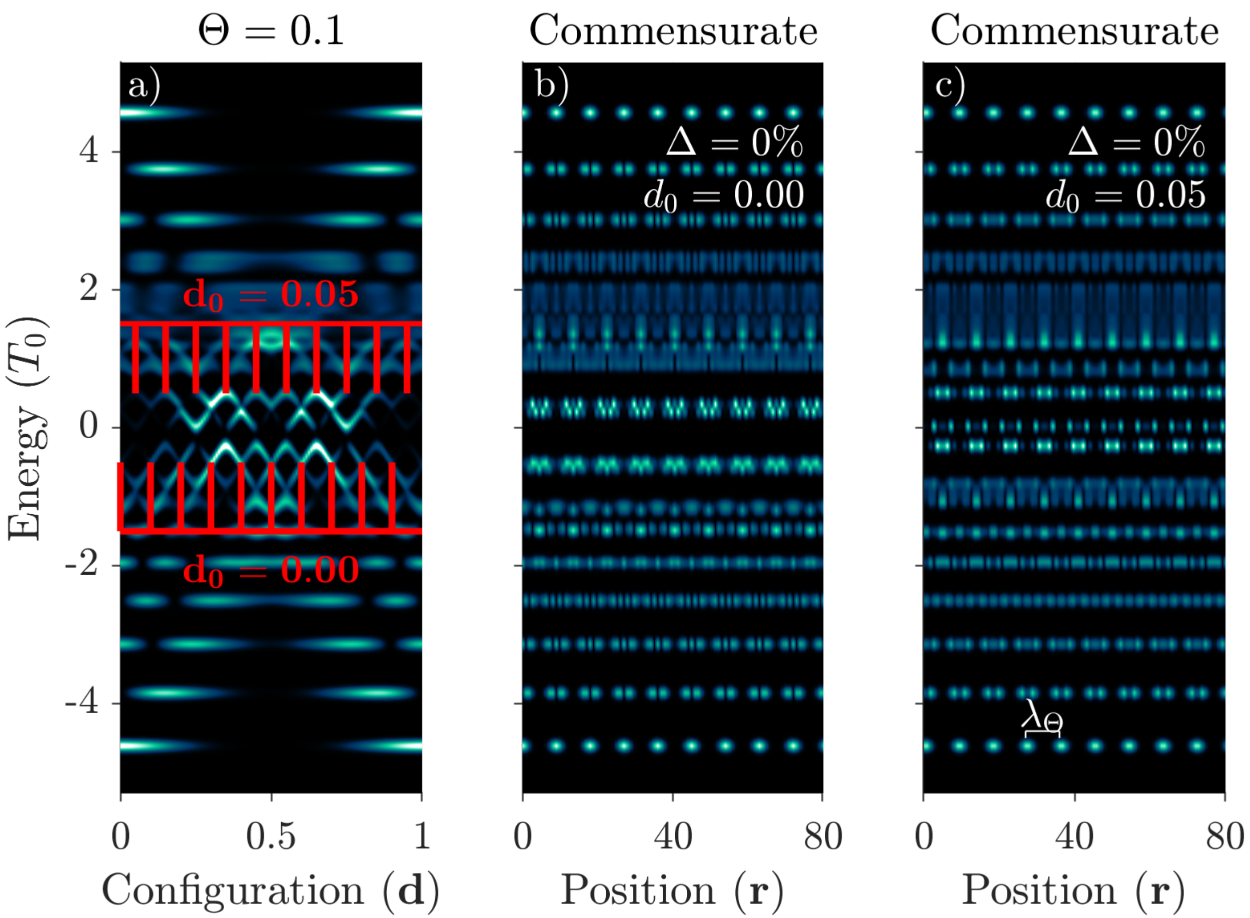
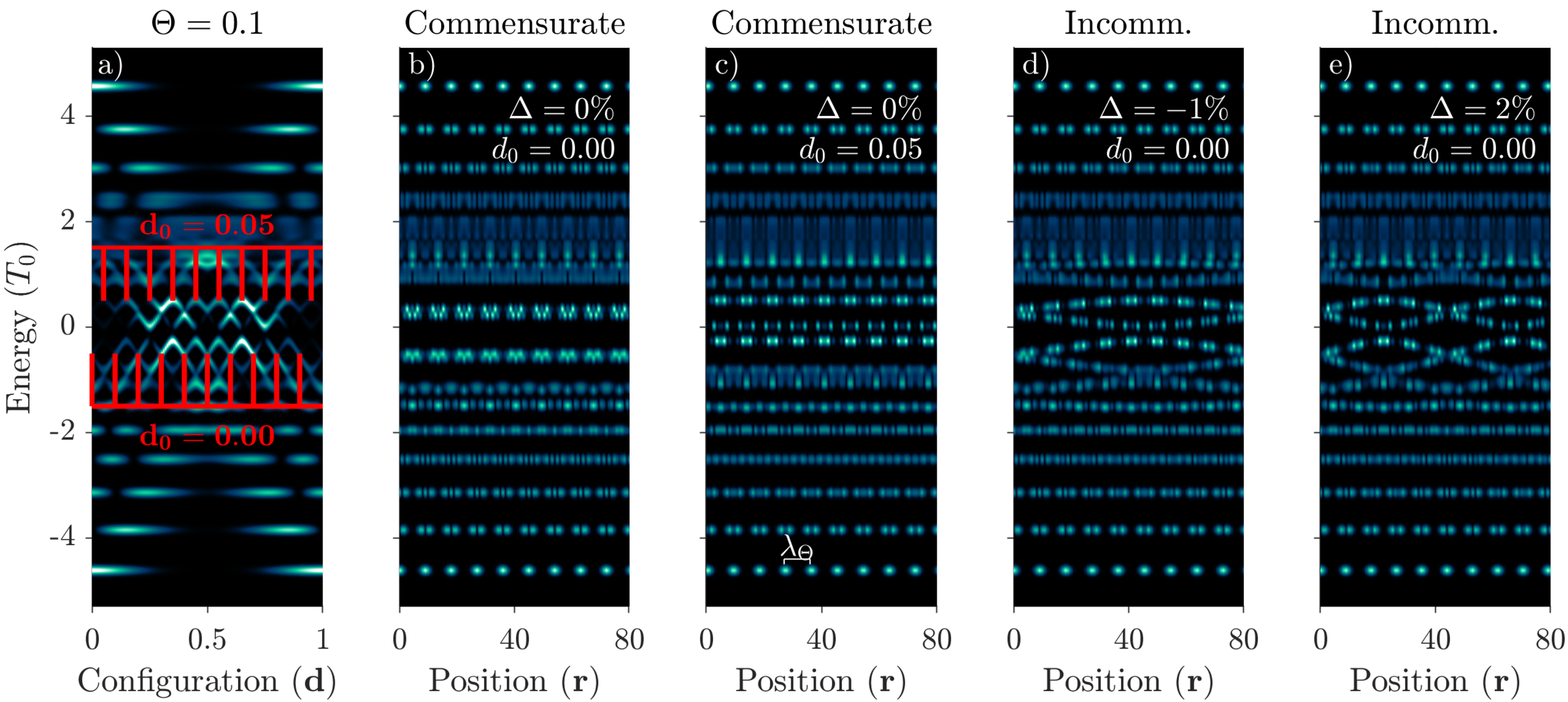


Incommensuration parameter:

$$\Theta = \Theta_0 \times (1 + \Delta)$$

Momentum crystal in real-space

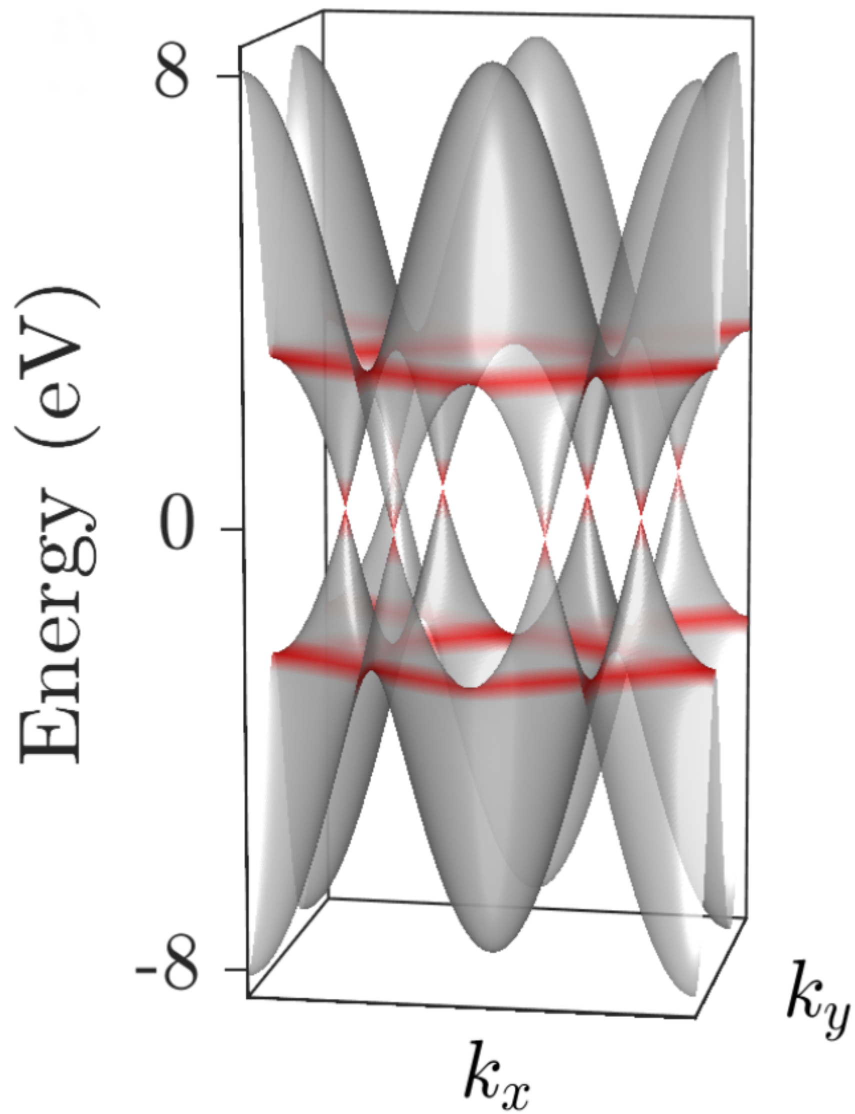


Incommensuration parameter:

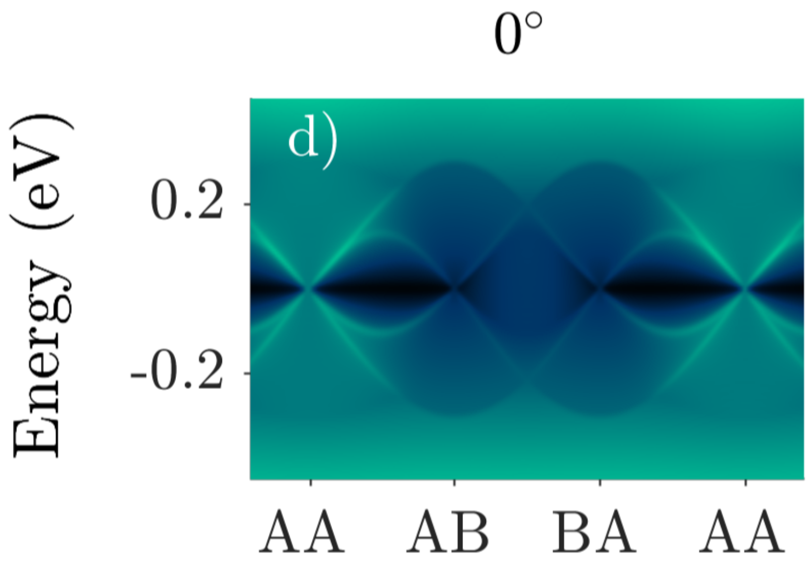
$$\Theta = \Theta_0 \times (1 + \Delta)$$

Momentum Crystal is analogous to the localization of a 1D TBH in an incommensurate potential

2D Example: Bilayer Graphene



Twistronic graphene, through LDoS



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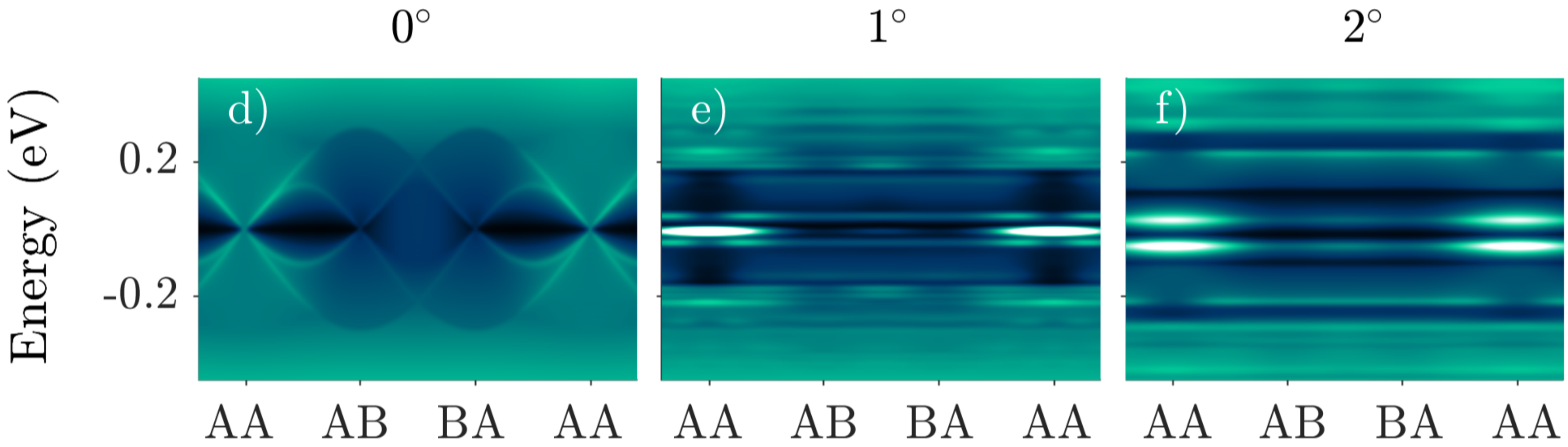
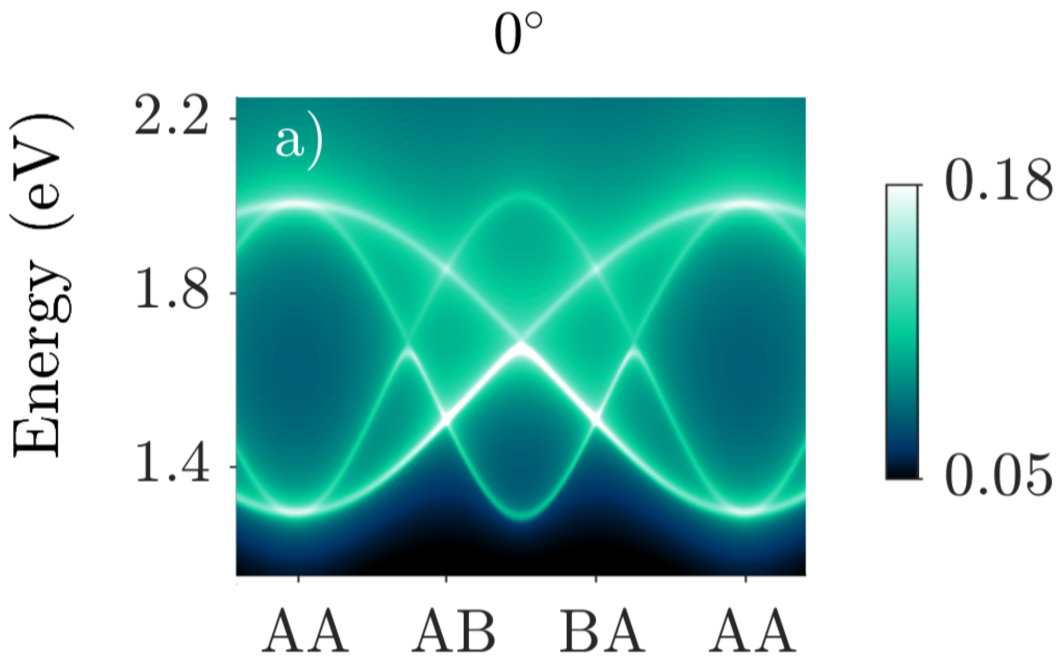
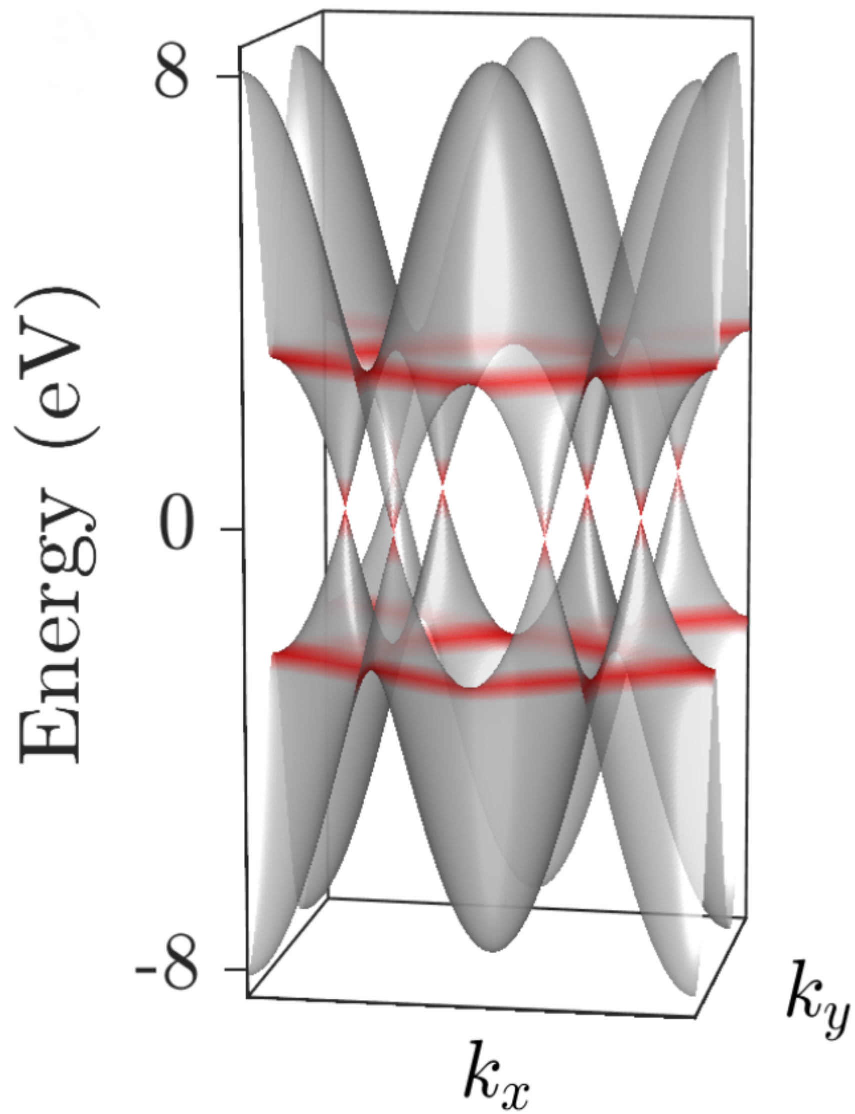


Large DOS enhancements at AA stacking
For low-energy TBG, bands are likely a better approach!

What about high energy?

Twistronic graphene, through LDoS





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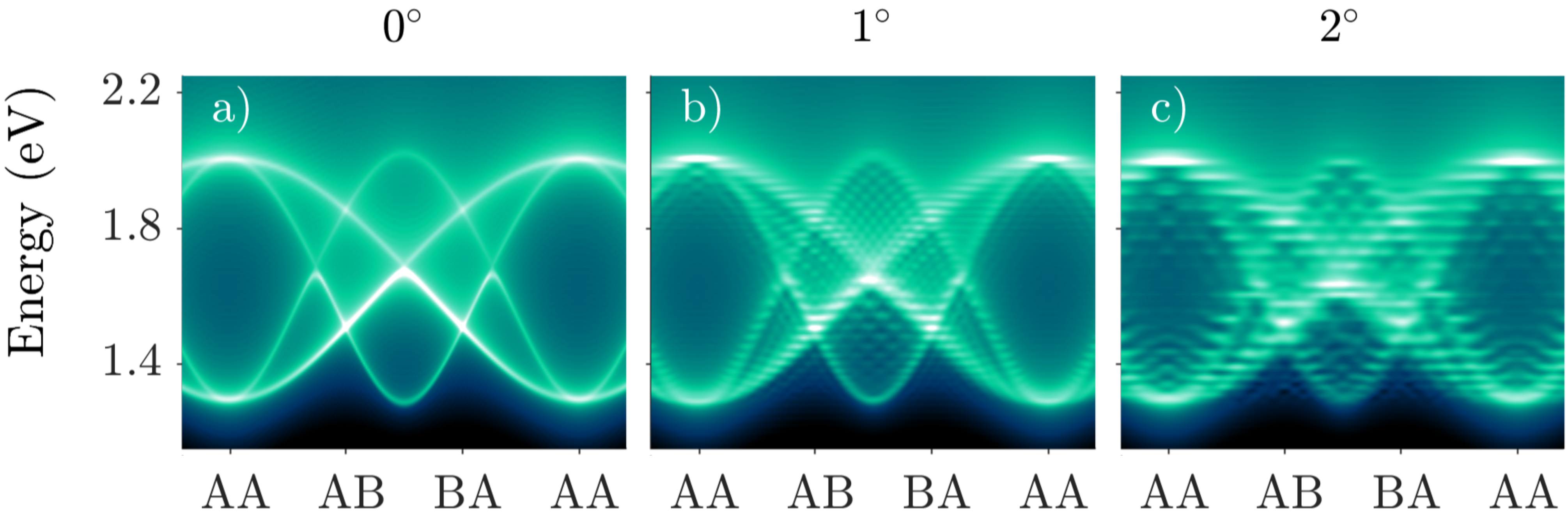
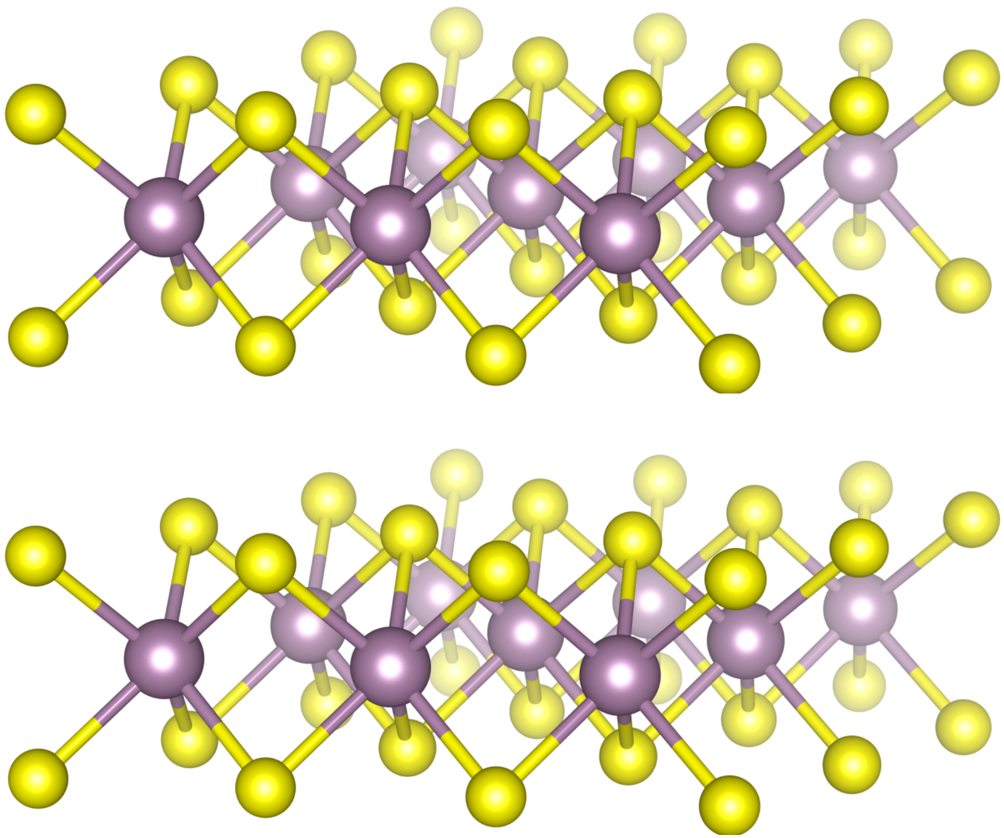
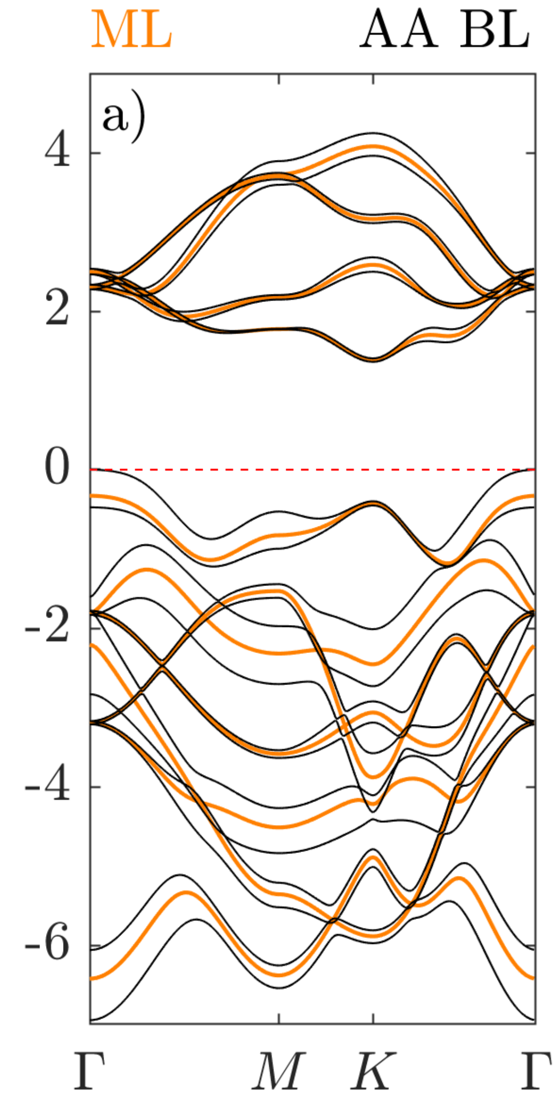


Lots of confined modes in metallic background, even above “magic angle”
No transport… but possible optical experiments (exciton spectrum?)

2D Example: Bilayer MoS_2





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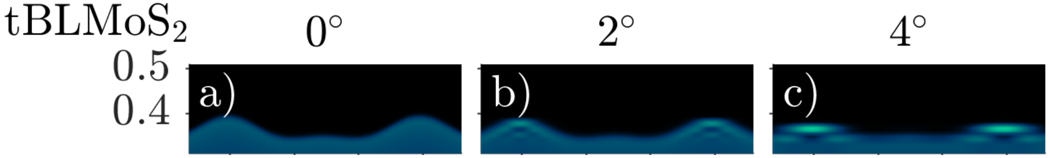

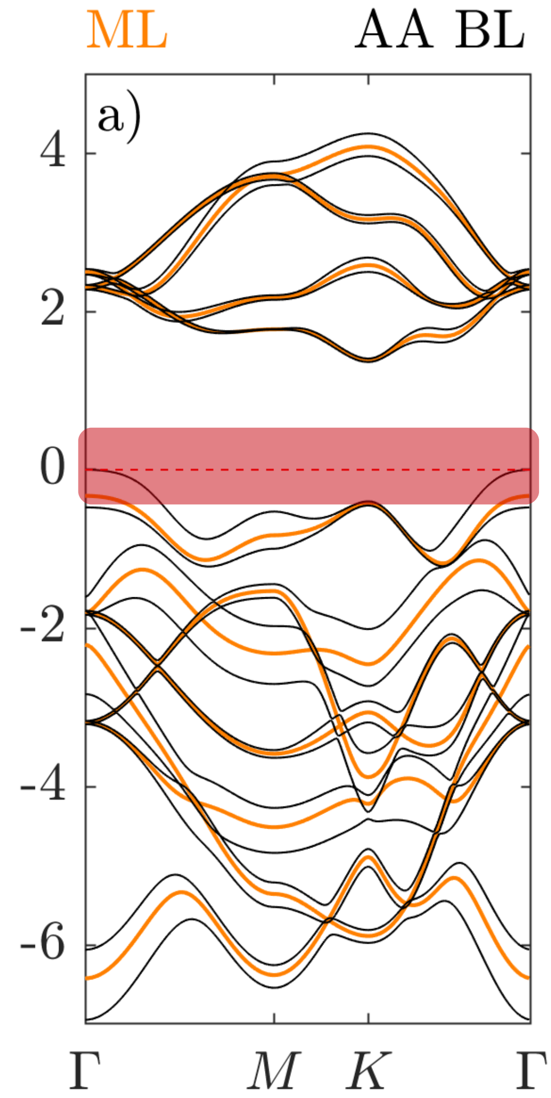

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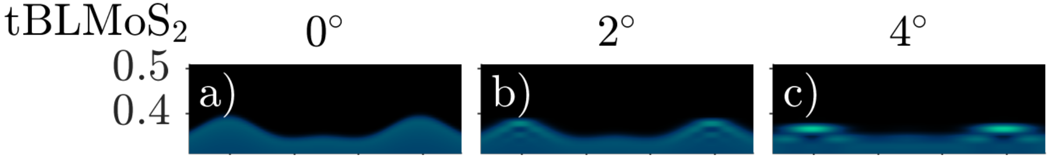
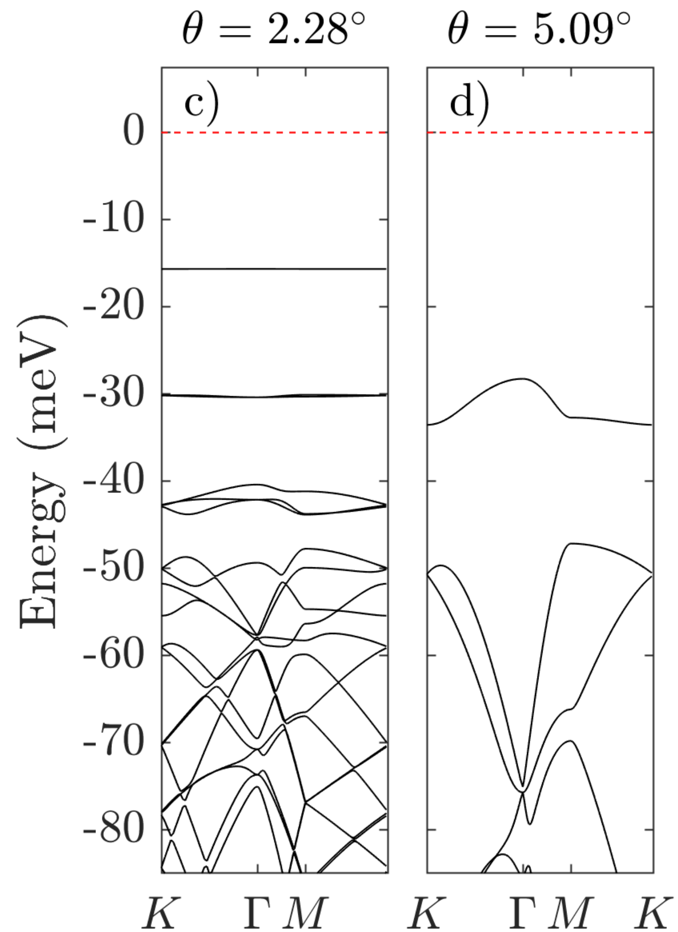


Tight-binding supercells



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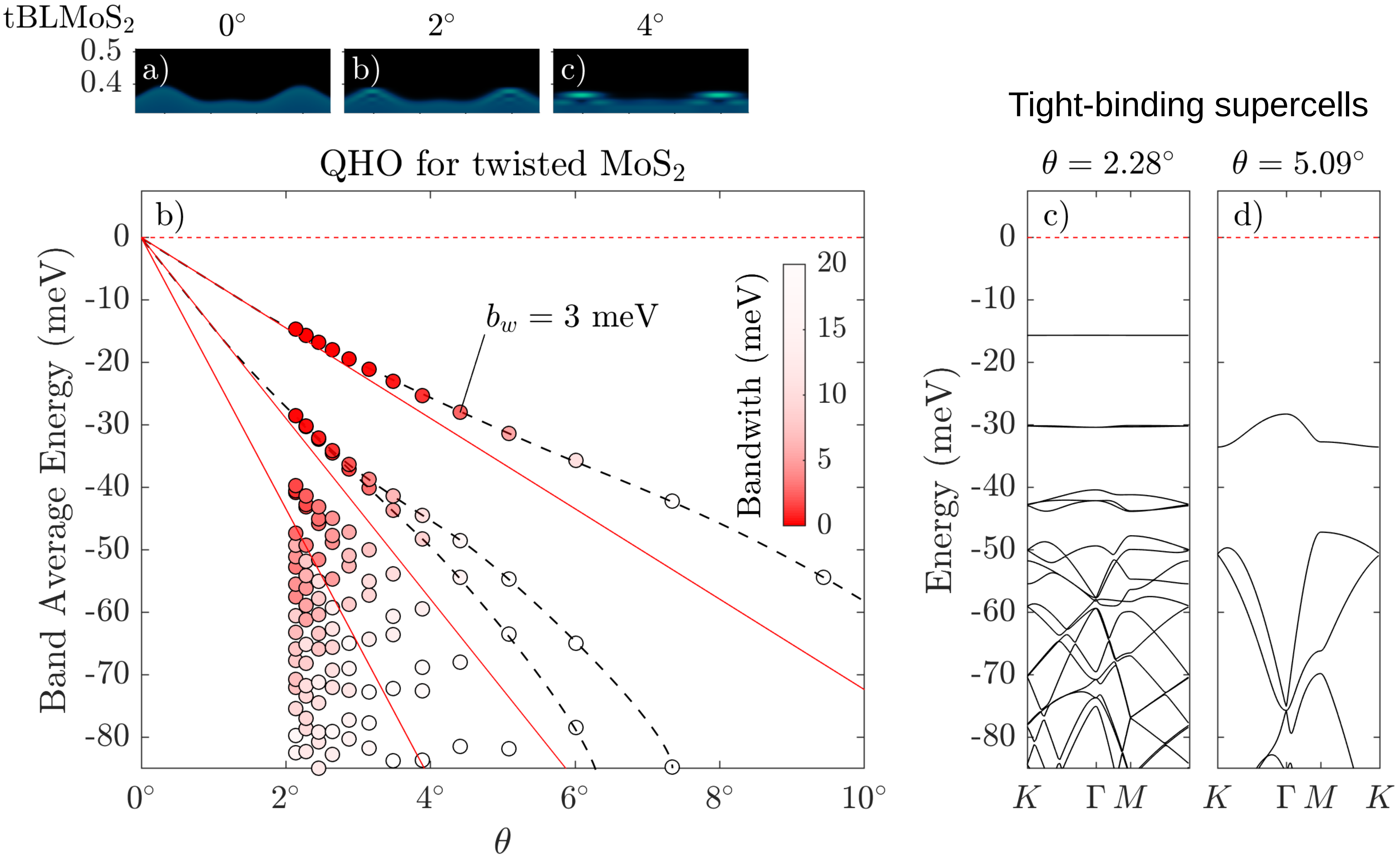

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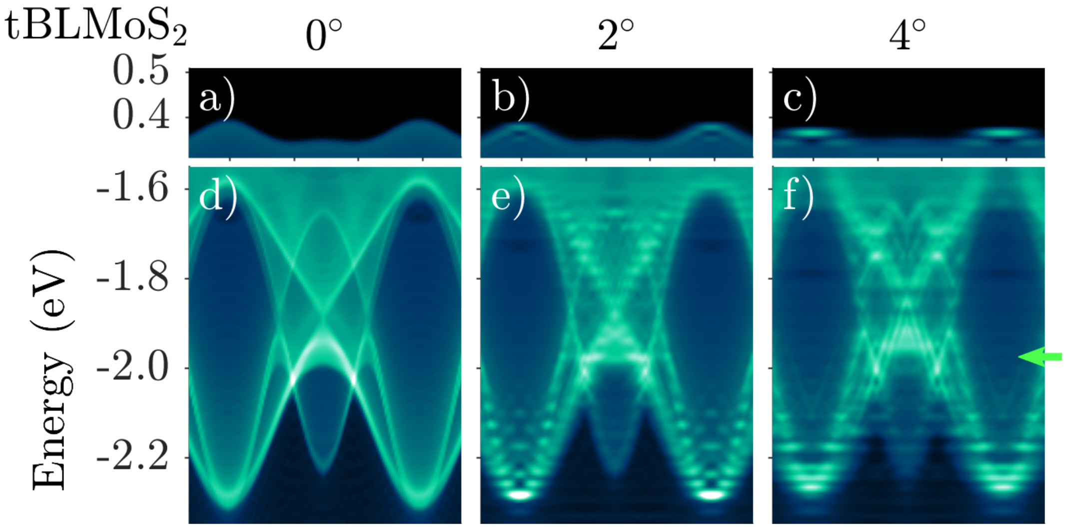

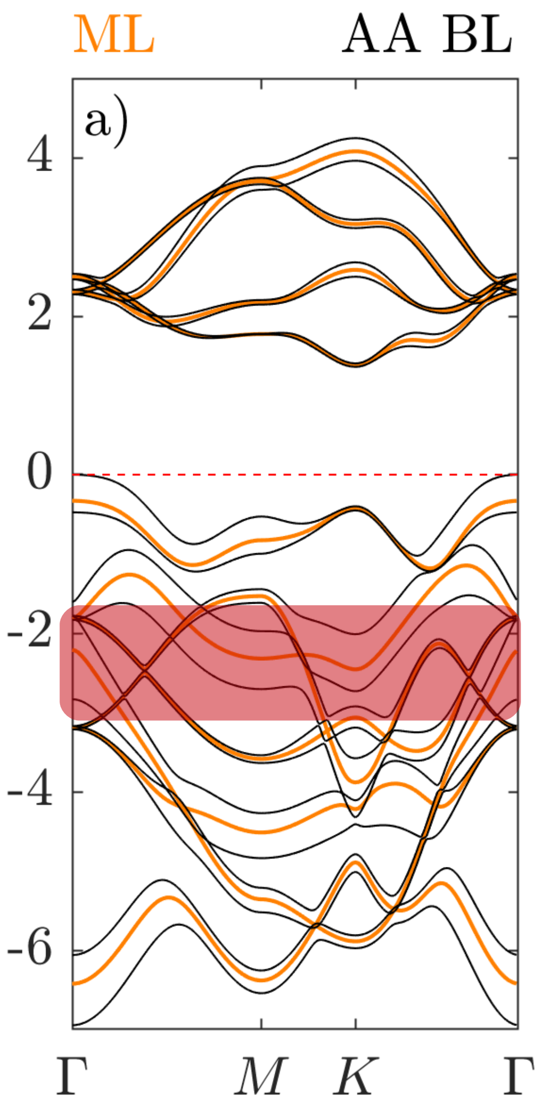

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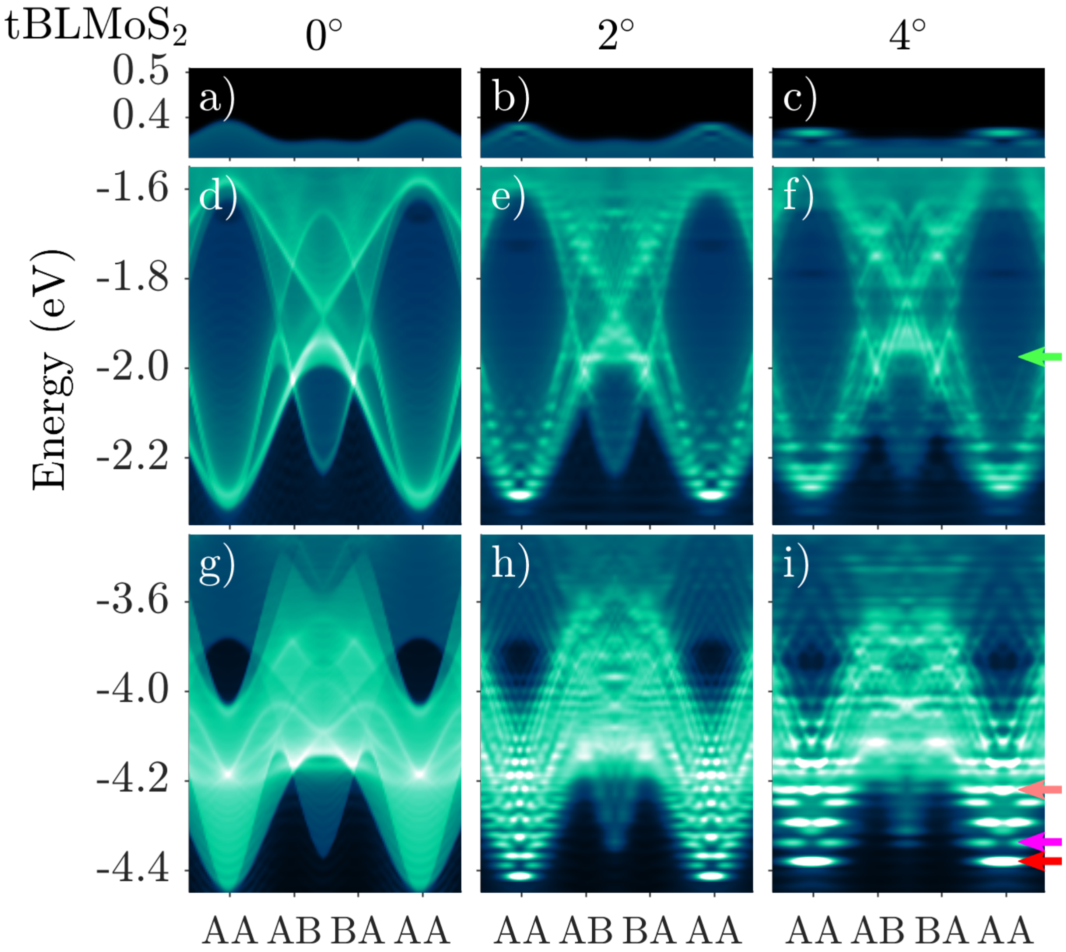

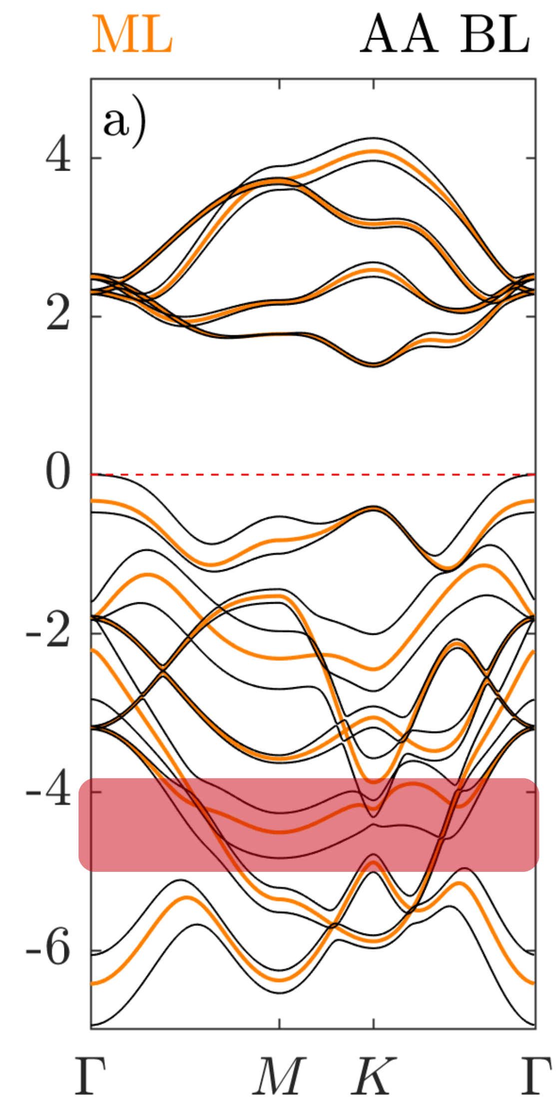

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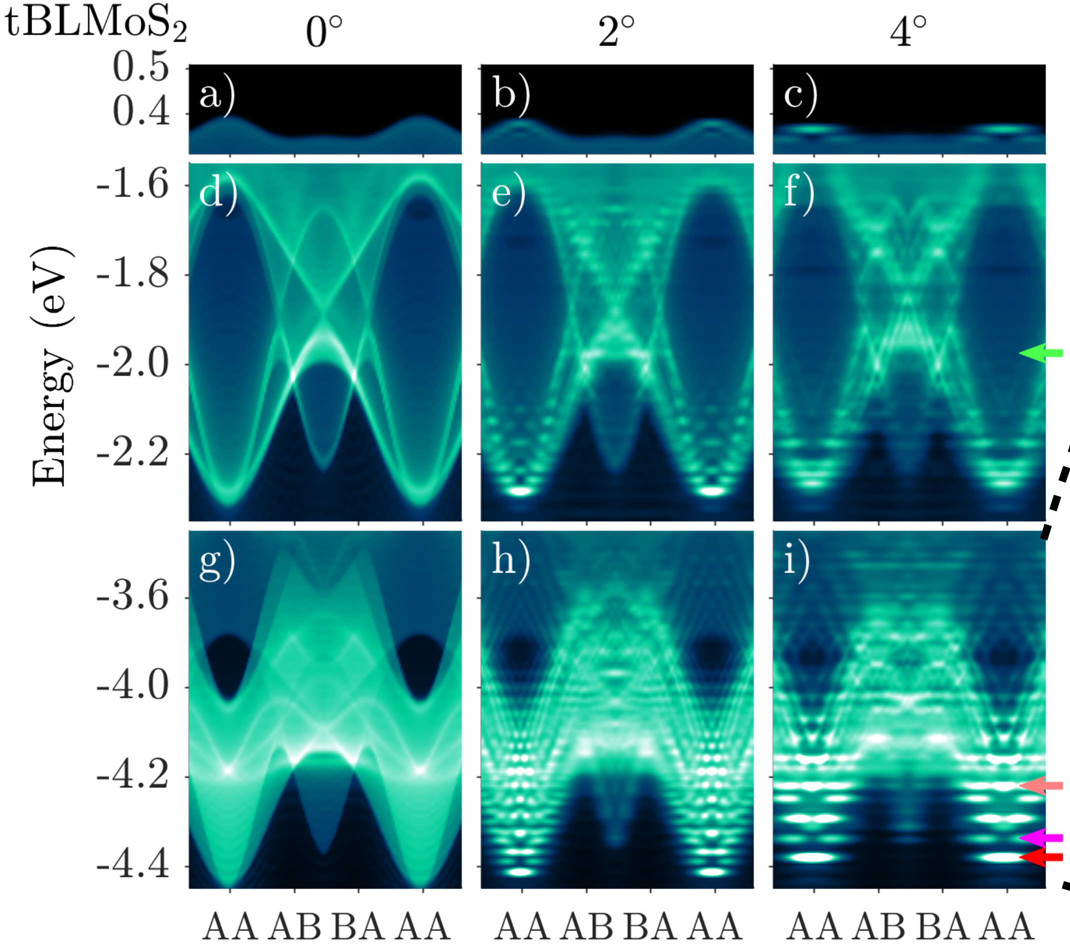

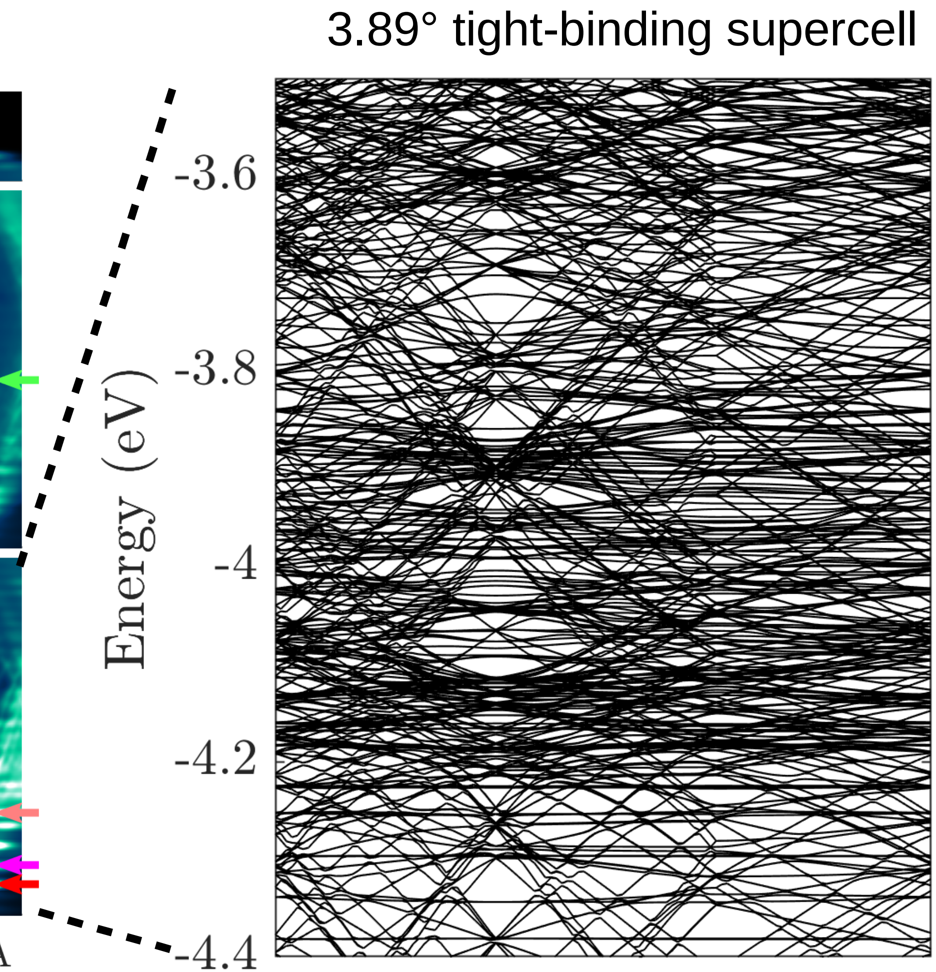

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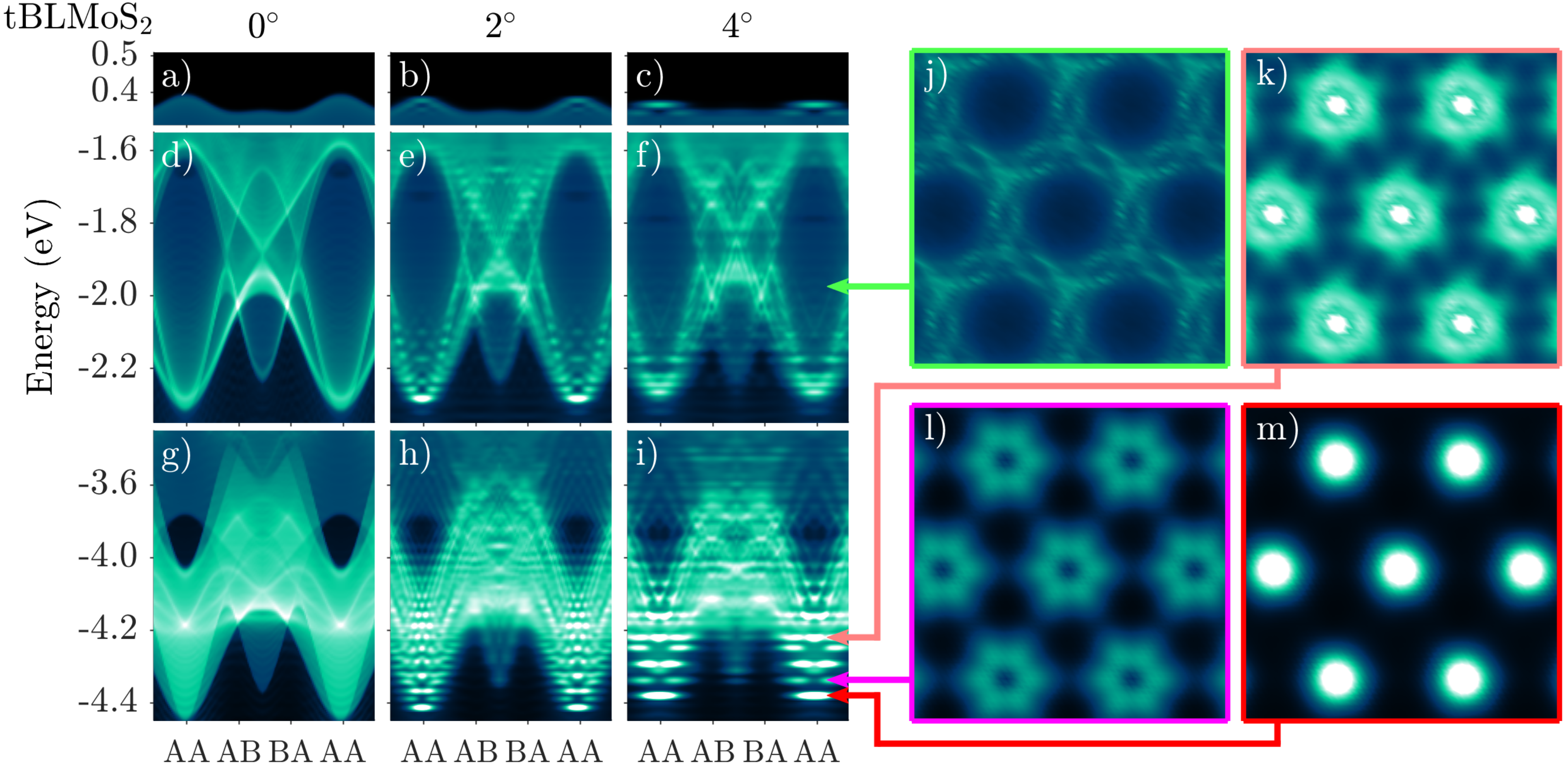


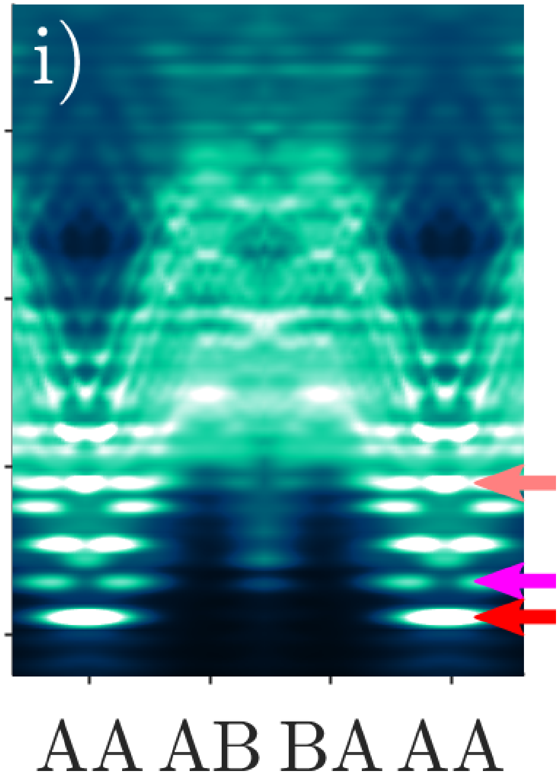
Summary

1) Introduced a framework for predicting moire electronic effects

2) Explored microscopic details of twistronics

3) Momentum-configuration duality in twisted bilayers

4) Studied examples in realistic 2D systems



- Look for simultaneous flat bands
- Metallic systems with flat bands
- Observable momentum crystal
- “By eye” predictions (machine learning?)

Acknowledgements

Efthimios Kaxiras
Shiang Fang
Zoe Zhu

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