Electric Field Tunable Band Gap
in Commensurate Twisted Bilayer Graphene

APS Mid-Atlantic Section Meeting • 2 December 2022

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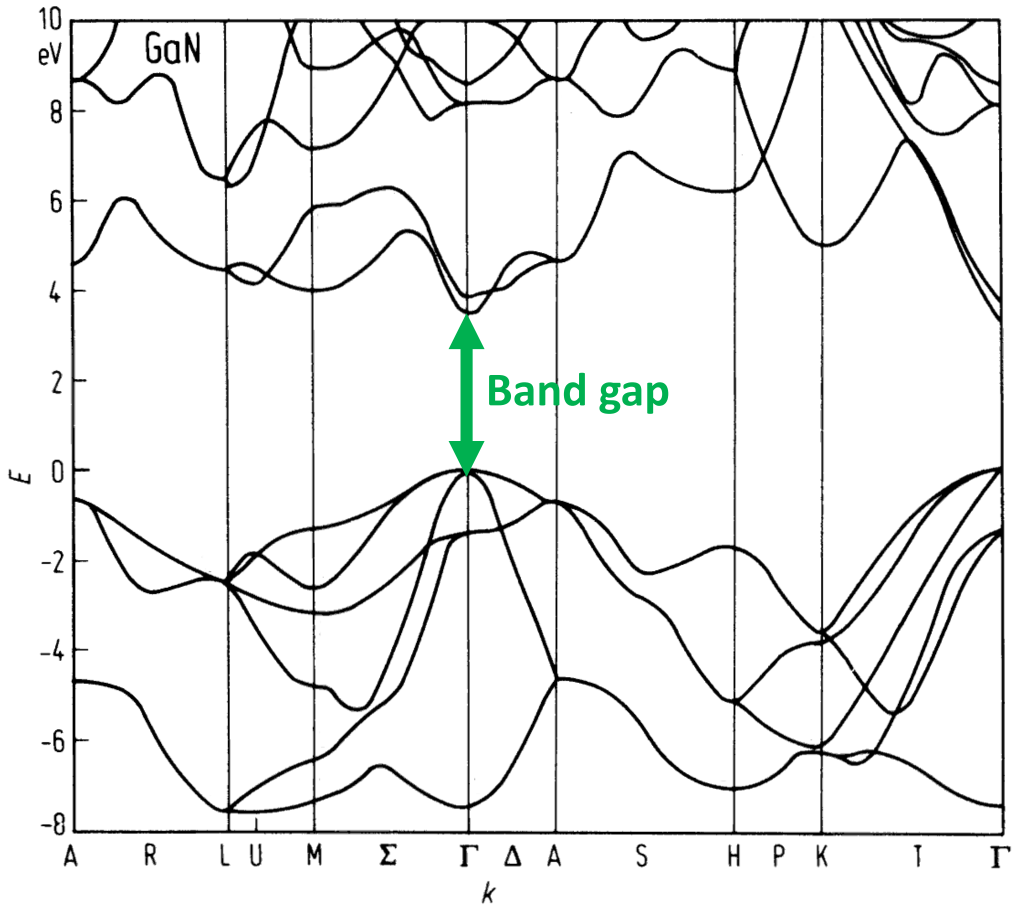
Semiconductors and Band Gaps

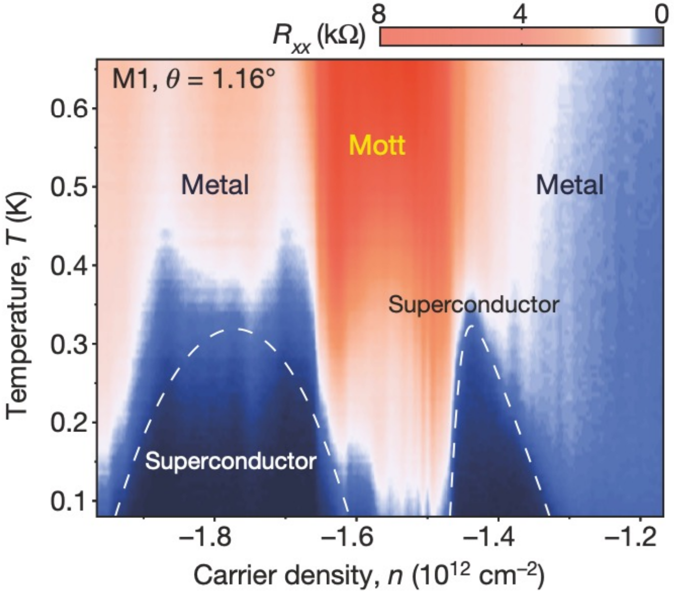
- Semiconductors are ubiquitous in modern technologies from information processing to lighting
- Key feature: band gap between valence and conduction electrons
- How can you change the band gap?
  - Usually you can't: n or p dope
- Bernal graphite bilayer
  - Apply E field to change gap



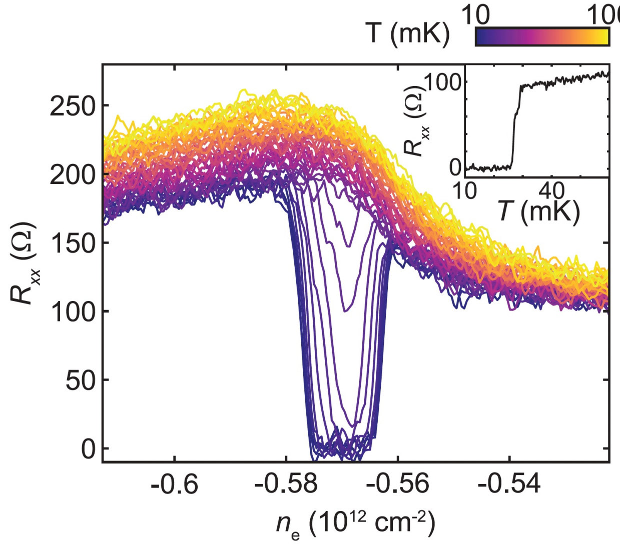
Phys. Stat. Solidi **66**, 161 (1974)

Twisted Bilayer Graphene

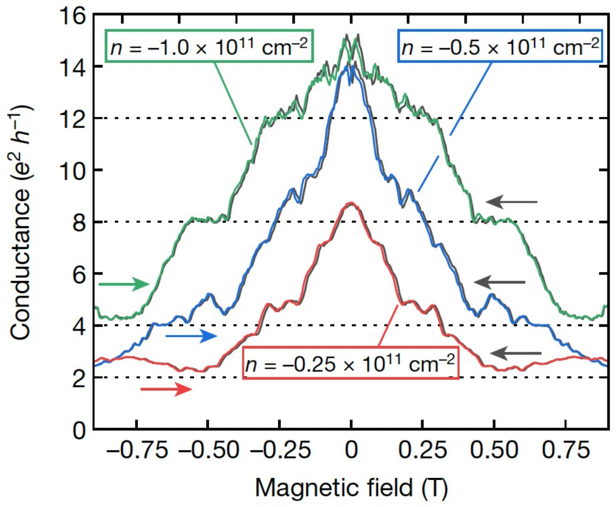
- Interesting physics at small angles
  - Flat bands --> many correlated states
  - Superconductivity, and much more
- Interesting physics at large angles
  - Dispersive bands --> no correlated states?
  - Still get superconductivity! And QAHE



Nature **556**, 43 (2018)



Science **375**, 774 (2022)



Nature **598**, 53 (2021)

Commensuration

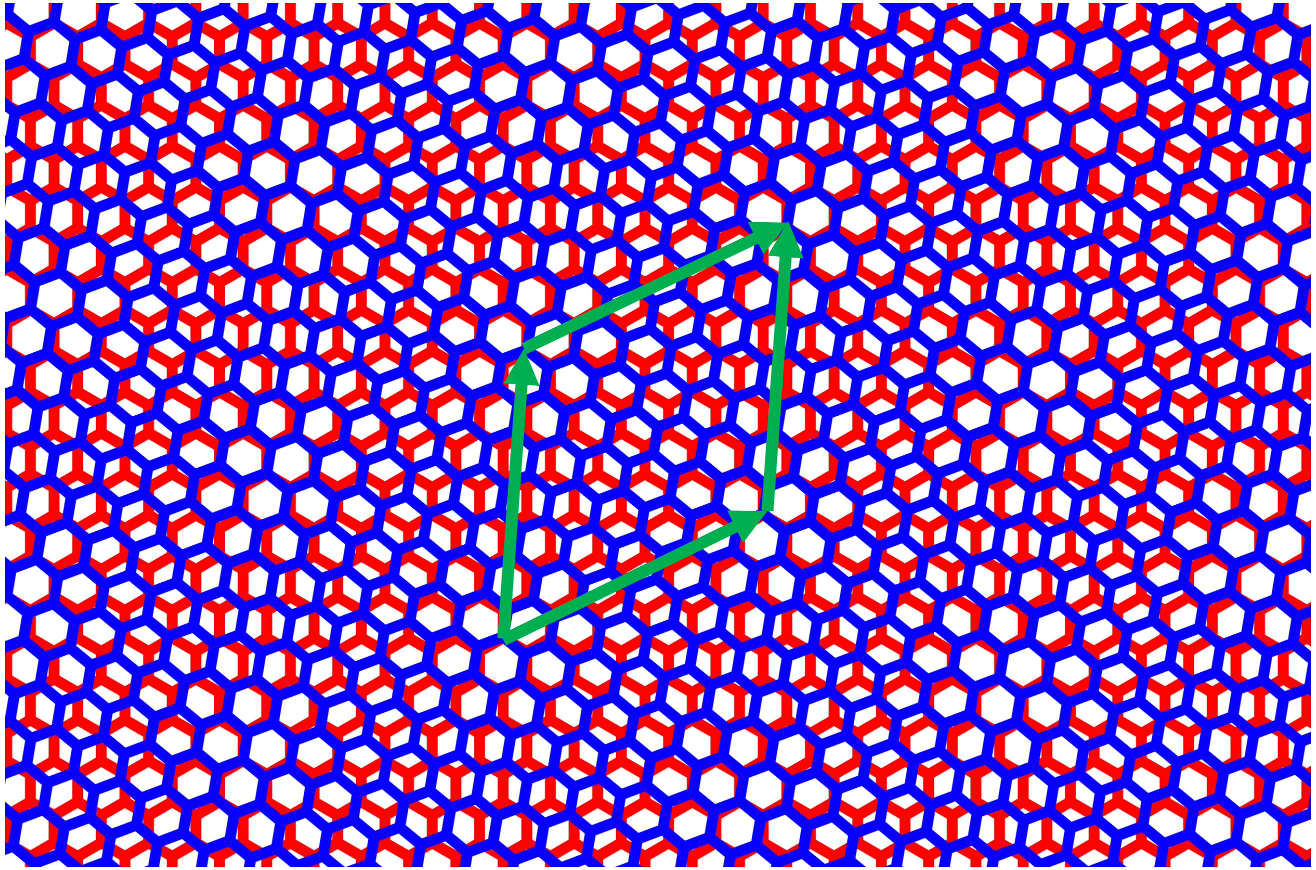
- Structures that are periodic in space are commensurate
- Commensuration condition

$$\theta(m,n) = \mathrm{Arg}\left[\frac{me^{-i\pi/6} + ne^{i\pi/6}}{ne^{-i\pi/6} + me^{i\pi/6}}\right]$$

- Small unit cells can occur
  - (1,2) and (1,4)

    $\sqrt{7}a \times \sqrt{7}a$
  - (1,3) and (2,5)

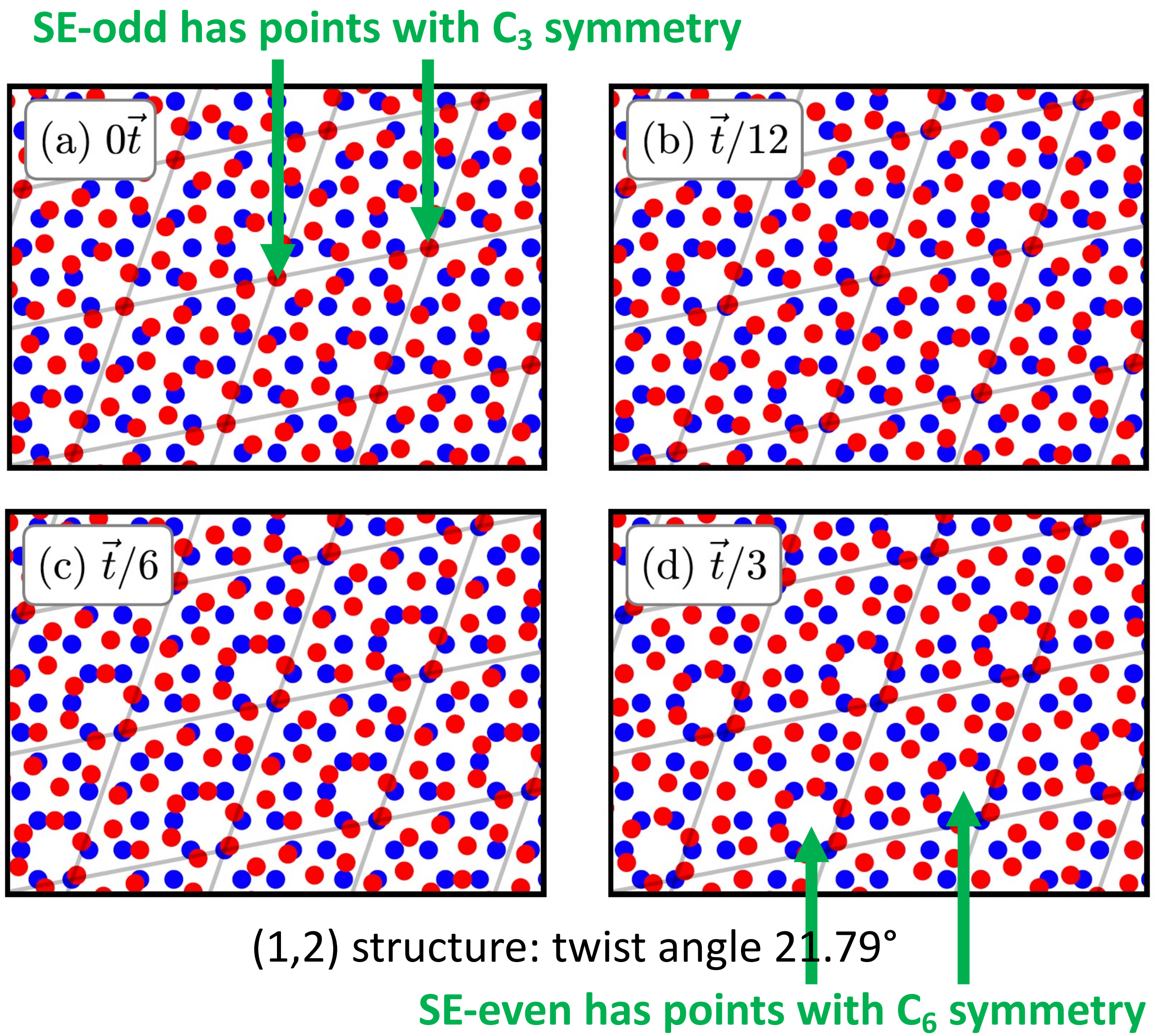
    $\sqrt{13}a \times \sqrt{13}a$



(4,3) structure: twist angle 9.43°

Slip and Sublattice-Exchange Symmetry

- Degrees of freedom in rigid sheets
  - Twist angle
  - Interlayer translation (slip)
- System can be odd, even or neither under exchange of A and B sublattices (SE)
- Odd: SE is an inversion
  - E.g. Bernal (AB) stacked bilayer
- Even: SE is the identity
  - E.g. AA stacked bilayer

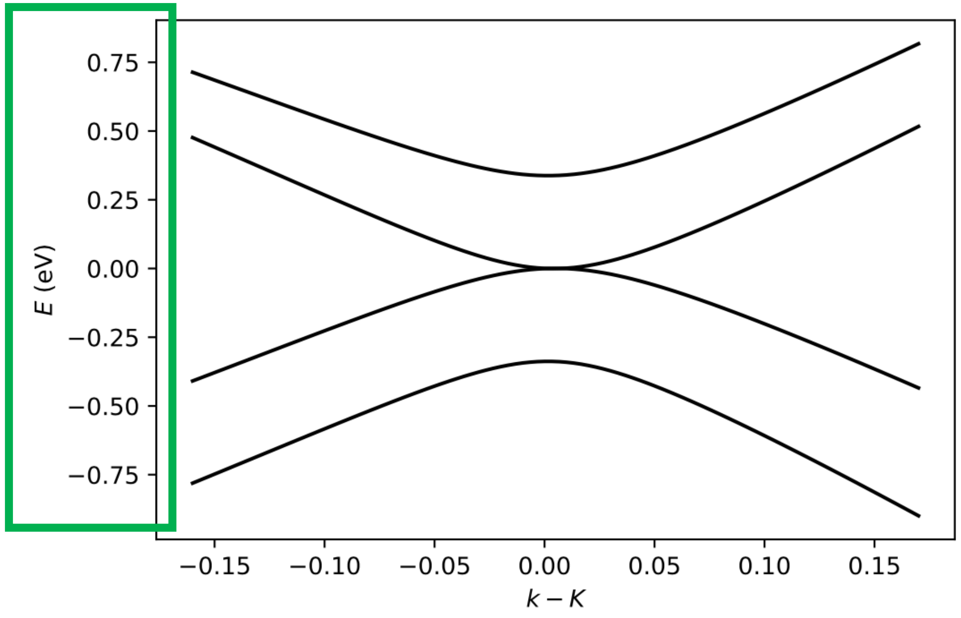


Inflated Unit Cells

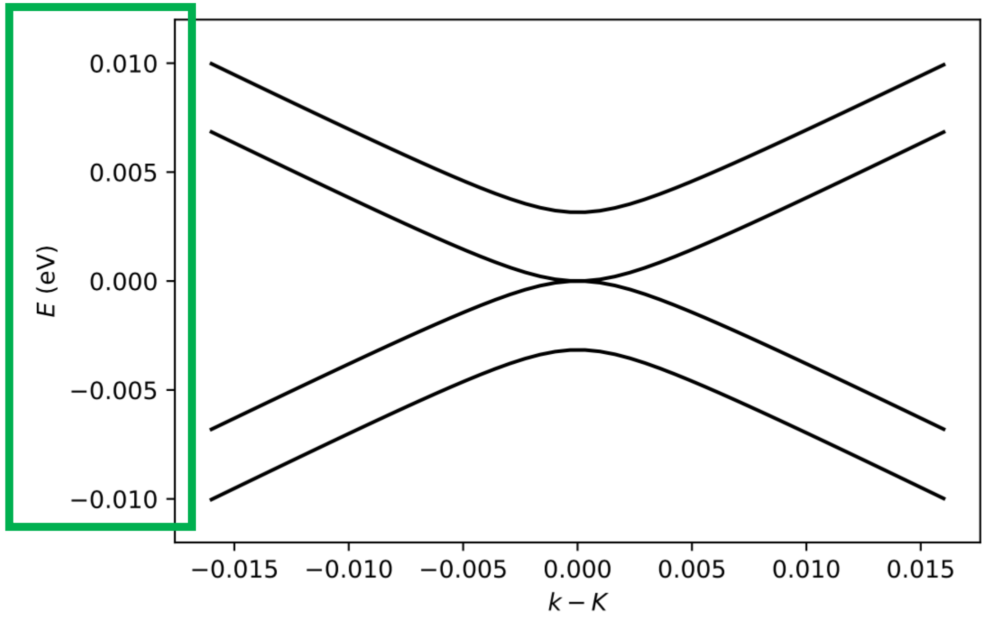
- Small unit cells exhibit low energy behavior analogous to the Bernal and AA structures but “inflated”

- Smaller Brillouin zone
- Smaller energy scales
- Smaller effective mass

Bernal structure



(1,2) structure



Symmetry Based Low Energy Theory

- Combining the relevant degrees of freedom one can obtain a low energy continuum model
- Expand about the K point
- Mele did this in PRB **81**, 161405 (2010)

$$H_{\boldsymbol{k}}^{\text{odd}} = \begin{pmatrix} \mathcal{E} & k_x - ik_y & V_0 & 0 \\ k_x + ik_y & \mathcal{E} & 0 & 0 \\ V_0 & 0 & -\mathcal{E} & -e^{i\theta}(k_x + ik_y) \\ 0 & 0 & -e^{-i\theta}(k_x - ik_y) & -\mathcal{E} \end{pmatrix}$$

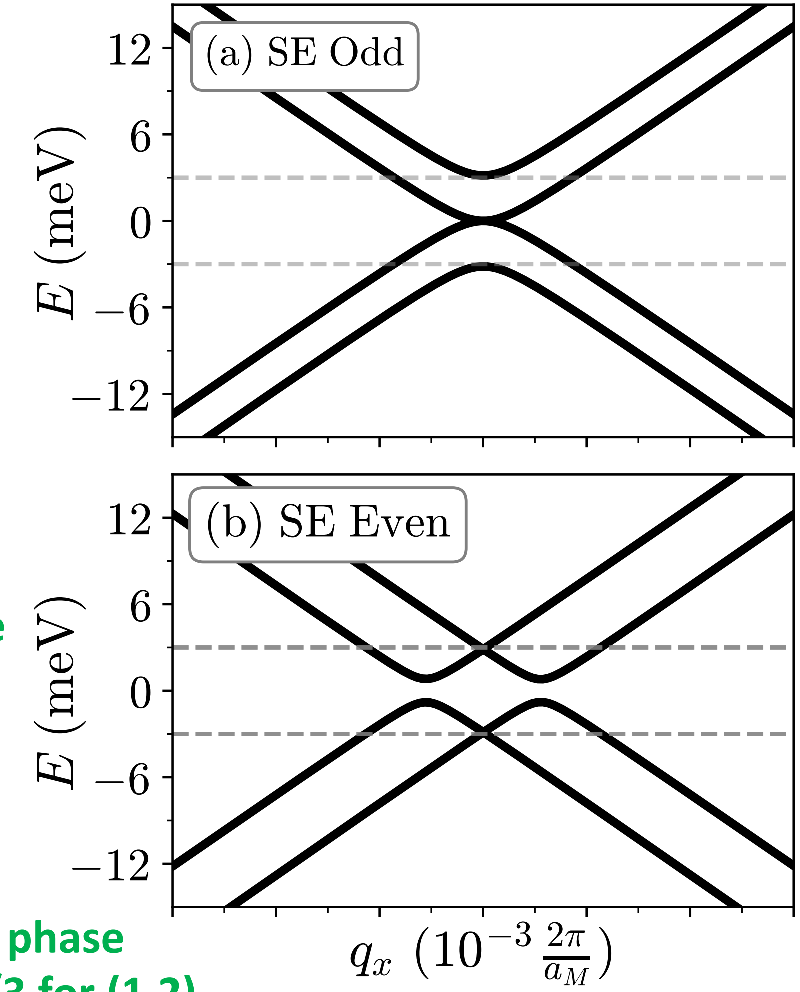
$$H_{\boldsymbol{k}}^{\text{even}} = \begin{pmatrix} \mathcal{E} & k_x - ik_y & V_0 e^{i\varphi/2} & 0 \\ k_x + ik_y & \mathcal{E} & 0 & V_0 e^{-i\varphi/2} \\ V_0 e^{-i\varphi/2} & 0 & -\mathcal{E} & e^{-i\theta}(k_x - ik_y) \\ 0 & V_0 e^{i\varphi/2} & e^{i\theta}(k_x + ik_y) & -\mathcal{E} \end{pmatrix}$$

Interlayer coherence

Twist angle

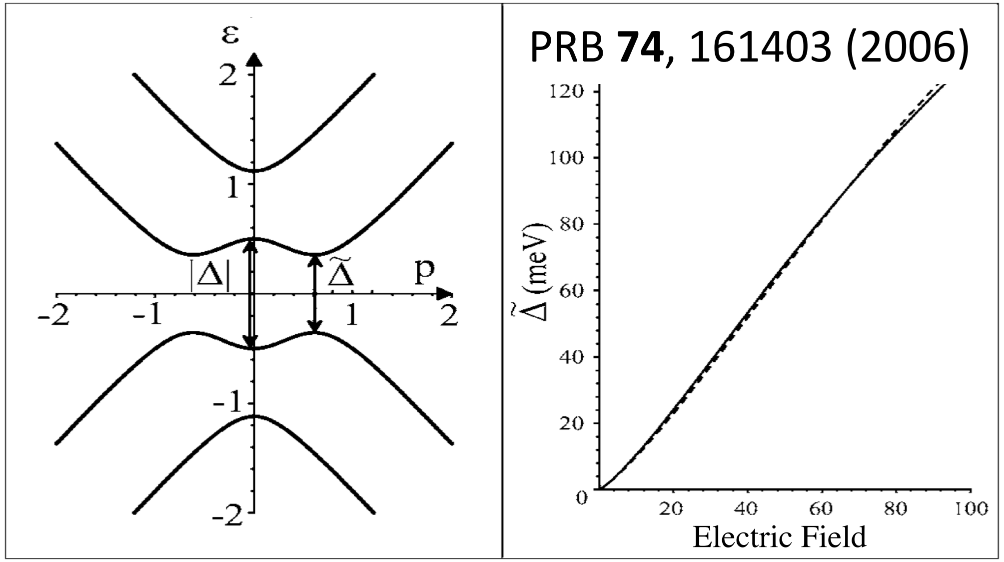
E field

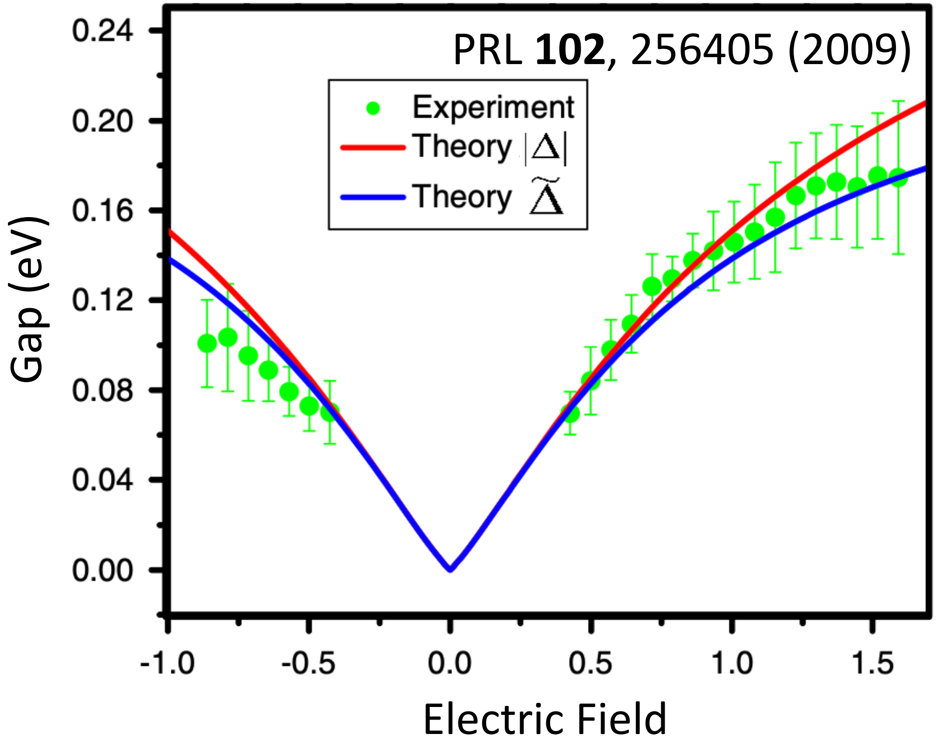
Pseudospin phase
0 for AA, π/3 for (1,2)



E-Field Tunable Band Gap of the Bernal Bilayer

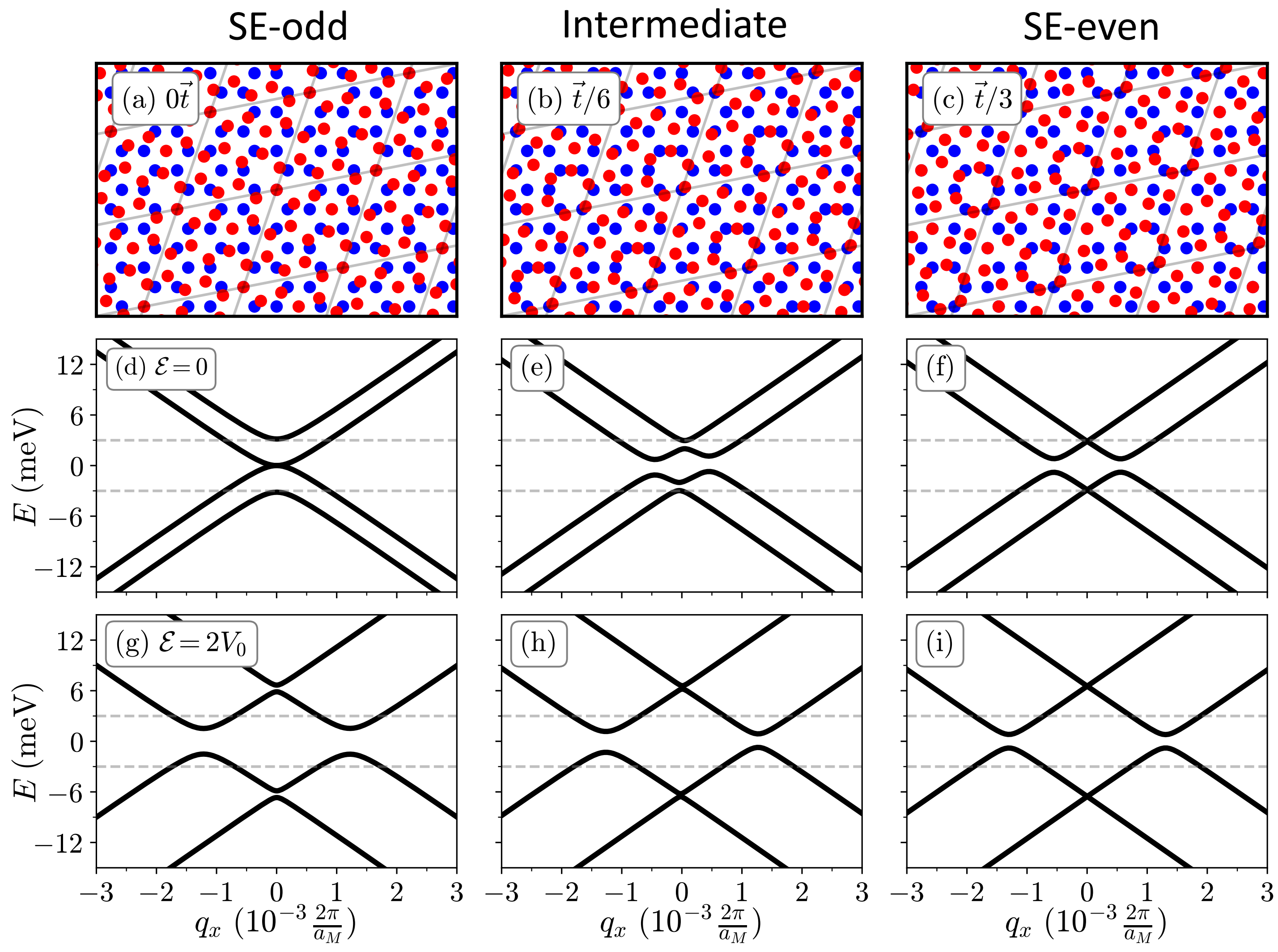
- Perpendicular E field leads to different potential energies in the layers
- Parity breaking lifts the quadratic band crossing the of Bernal bilayer
- Band gap is tunable through the IR





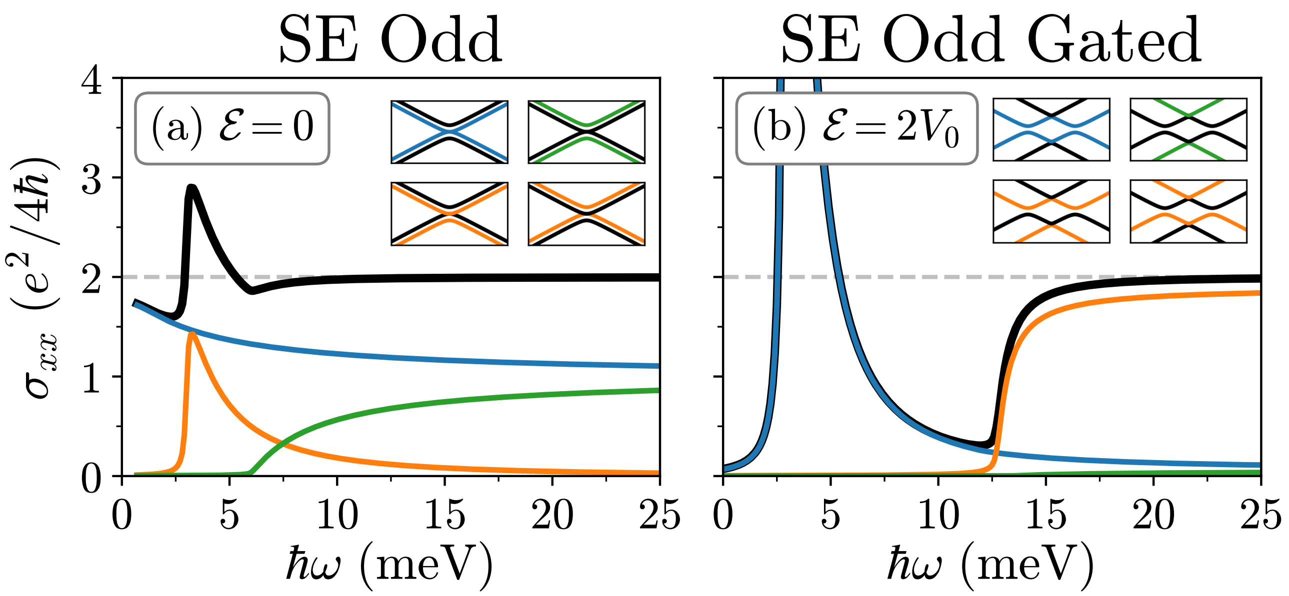
E-Field and Bands in Commensurate TBG

- E-field lifts band touching in SE-odd
- In large E-field SE-odd gap saturates to the interlayer coherence scale V_0
- SE-even gap is independent of E
- Remote bands decouple into two independent Dirac cones



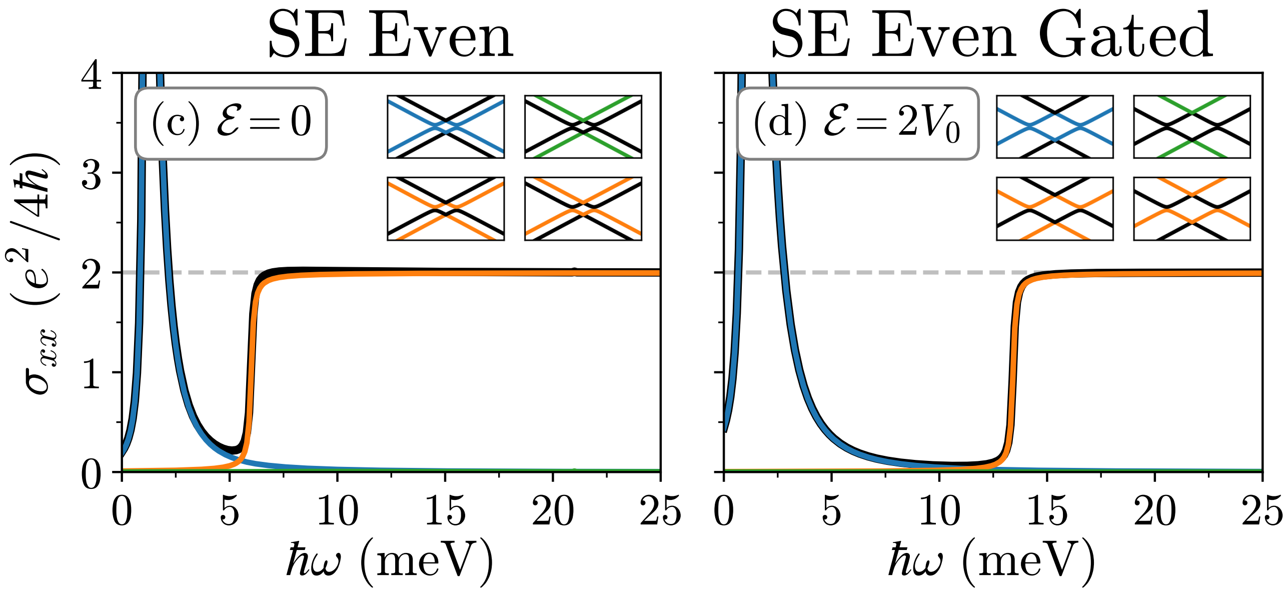
SE-Odd

- E-Field tunable band gap
- Interlayer coherence
  - Hybridizes the two Dirac cones near the Fermi energy
  - Dirac cones remain orthogonal far from the Fermi energy
    - Forbidden transitions



SE-Even

- Gap is independent of E-field
- Interlayer coherence
  - Hybridizes the two Dirac cones near the Fermi energy
  - Dirac cones remain orthogonal far from the Fermi energy
    - Forbidden transitions



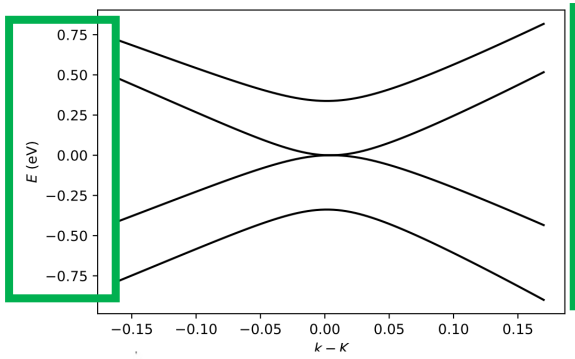
Comparison to the Bernal Bilayer

- Different saturation optical conductivities
  - 2 band model vs 4 band model in the THz
- Different approaches to gap saturation

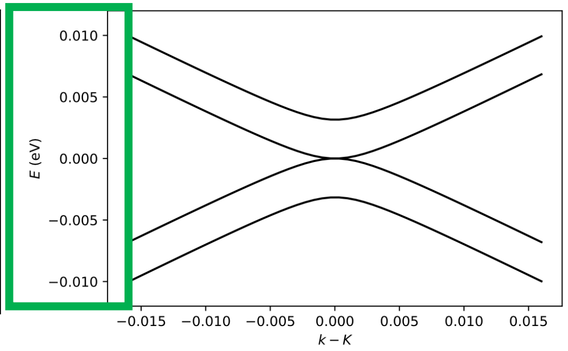
$$\widetilde{\Delta}(\mathcal{E}) = V_0\sqrt{\frac{4\mathcal{E}^2/V_0^2}{1+4\mathcal{E}^2/V_0^2}}$$

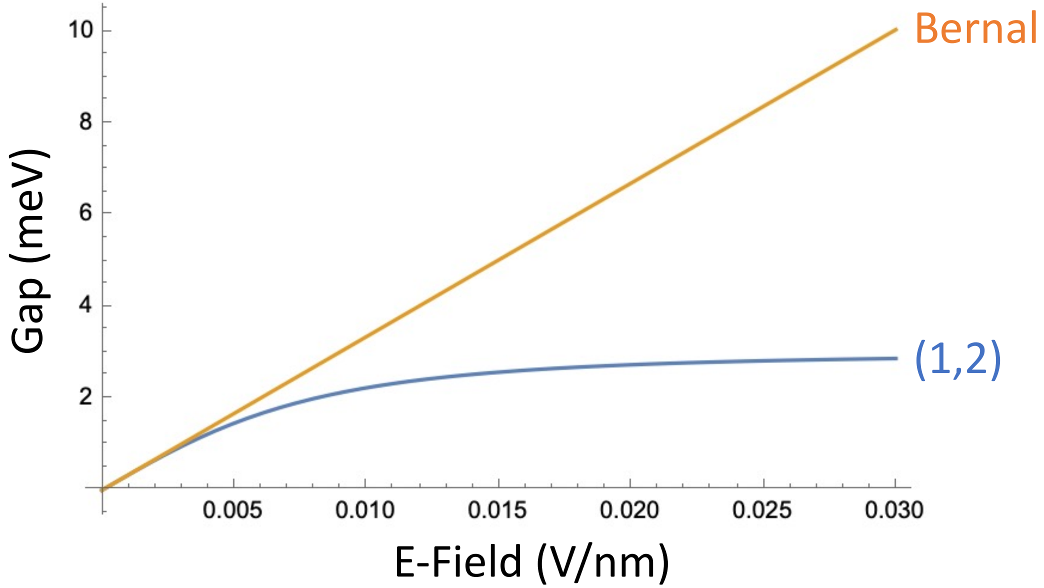
- Different interlayer coherences
  - V_0^{Bernal} = 338 meV
  - $V_0^{\text{SE-odd}}$ = 3 meV

Bernal structure



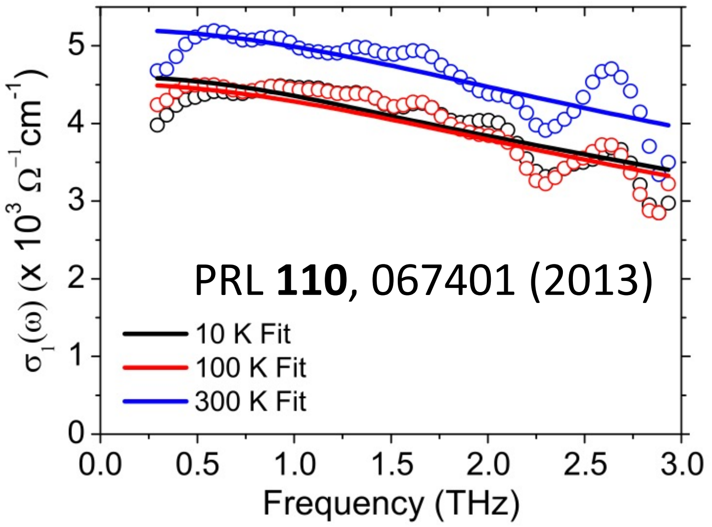
(1,2) structure





Outlook

- SE-odd and SE-even commensurate bilayers are “inflated” versions of Bernal and AA bilayers
- Take bands from eV scale to the THz / Coulomb energy scale: interactions will be interesting!
- Rich four-band models that are tunable with electrostatic gating for (1,2) and (1,4) structures
- First step: measure the interlayer coherence V_0



Uniform twist-angle samples

Peaks that probe the interlayer coherence scale

Acknowledgements

We thank the condensed matter group at UPenn and Pablo Jarillo-Herrero for discussions surrounding this work and acknowledge funding support from the NSF and DOE.

S.T. acknowledges support from the NSF under Grant No. DGE-1845298. E.J.M. acknowledges support from the DOE under Grant No. DE-FG02-84ER45118.

Kubo Formula Integration

- Kubo formula (non-interacting, non-relativistic, low temperature):

$$\sigma_{\mu\nu} = i\frac{e^2}{\hbar}\sum_{s,s'}\int_{\mathrm{BZ}}\frac{d\boldsymbol{k}}{(2\pi)^{\mathrm{dim}}}\frac{1}{\epsilon_{s'}-\epsilon_s}\frac{\langle s,\boldsymbol{k}|\hbar\hat{v}_\mu|s',\boldsymbol{k}\rangle\langle s',\boldsymbol{k}|\hbar\hat{v}_\nu|s,\boldsymbol{k}\rangle}{\hbar\omega-(\epsilon_{s'}-\epsilon_s)+i\eta}$$

- Velocity operators (in gradient approximation):

$$\hat{v}_\mu = \frac{\partial\mathcal{H}}{\partial k_\mu}$$