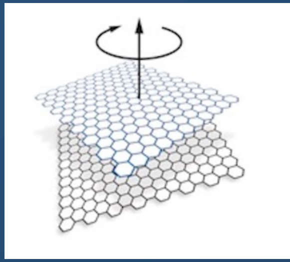
Superconductivity in twisted graphene layers: electronic structure and interactions.

Outline

- Superconductivity in twisted graphene bilayers.
- Electronic structure.
- Electrostatic interactions.
- Electron assisted hopping and superconductivity.
- Open challenges.

NANOCIENCIA

The University of Manchester



Correlations in Moire Flat Bands

F. Guinea

KITP, January 16th, 2019

In colaboration with N. R. Walet, U. Manchester
Acknowledgments to P. San Jose and J. Gonzalez, CSIC, Madrid.

Superconductivity in graphene

Superconductivity in graphene. March Meeting, Los Angeles 2018

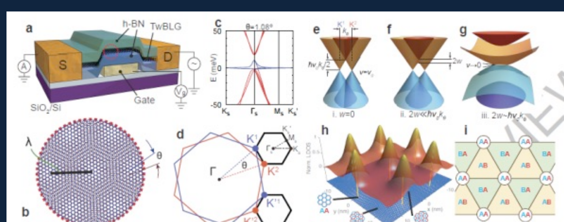
nature Accelerated Article Preview

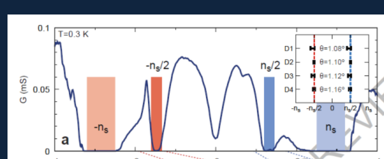
LETTER

doi:10.1038/nature26154

Correlated insulator behaviour at half-filling in magic-angle graphene superlattices

Yuan Cao, Valla Fatemi, Ahmet Demir, Shiang Fang, Spencer L. Tomarken, Jason Y. Luo, J. D. Sanchez-Yamagishi, K. Watanabe, T. Taniguchi, E. Kaxiras, R. C. Ashoori & P. Jarillo-Herrero





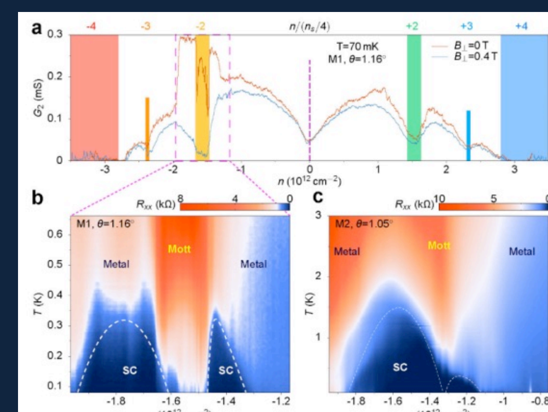
nature Accelerated Article Preview

ARTICLE

doi:10.1038/nature26160

Unconventional superconductivity in magic-angle graphene superlattices

Yuan Cao, Valla Fatemi, Shiang Fang, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras & Pablo Jarillo-Herrero

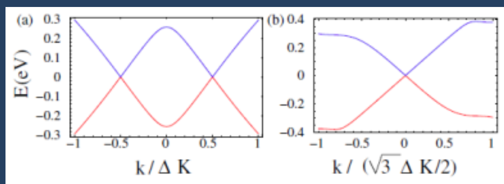


Twisted graphene layers: theory

PRL 99, 256802 (2007) PHYSICAL REVIEW LETTERS week ending 21 DECEMBER 2007

Graphene Bilayer with a Twist: Electronic Structure

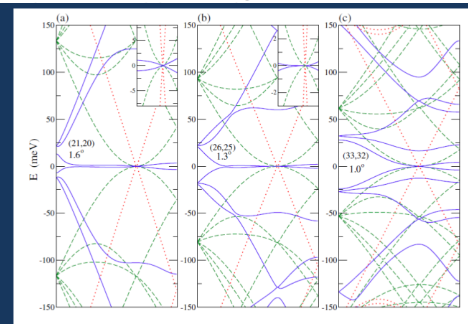
J. M. B. Lopes dos Santos,[1] N. M. R. Peres,[2] and A. H. Castro Neto[3]



PHYSICAL REVIEW B 82, 121407(R) (2010)

Flat bands in slightly twisted bilayer graphene: Tight-binding calculations

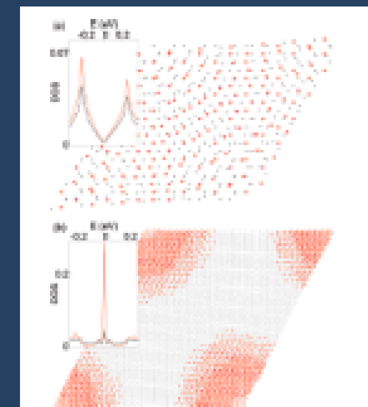
E. Suárez Morell, J. D. Correa, P. Vargas, M. Pacheco,* and Z. Barticevic



NANO LETTERS

Localization of Dirac Electrons in Rotated Graphene Bilayers

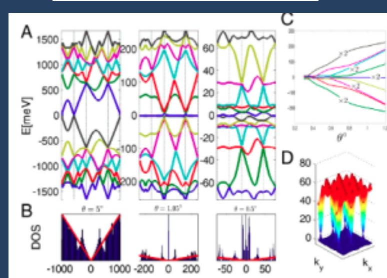
G. Trambly de Laissardière, D. Mayou, and L. Magaud



Moiré bands in twisted double-layer graphene

Rafi Bistritzer and Allan H. MacDonald[1]

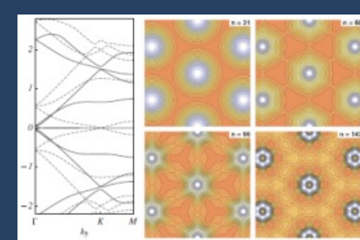
PNAS | July 26, 2011 | vol. 108 | no. 30 | 12233–12237



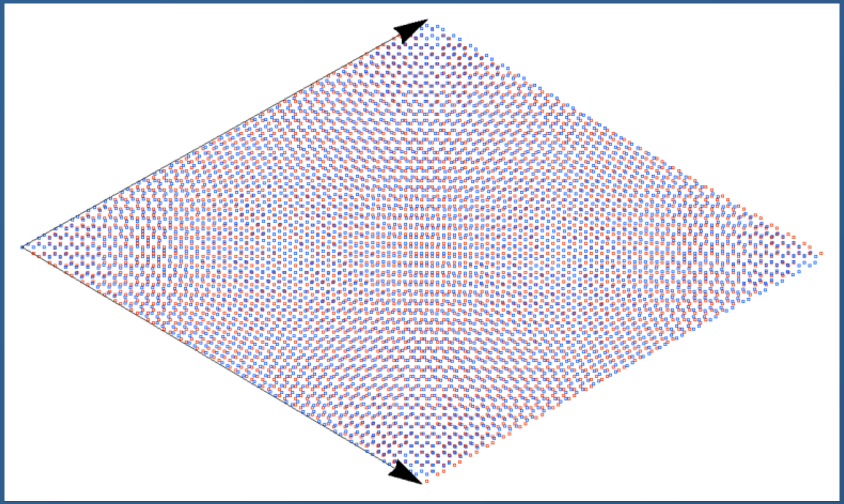
PRL 108, 216802 (2012) PHYSICAL REVIEW LETTERS

Non-Abelian Gauge Potentials in Graphene Bilayers

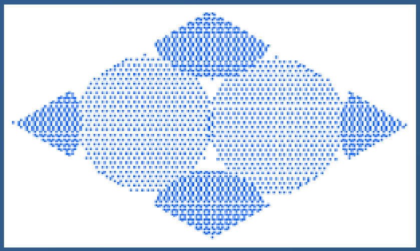
P. San-Jose,[1] J. González,[1] and F. Guinea[2]

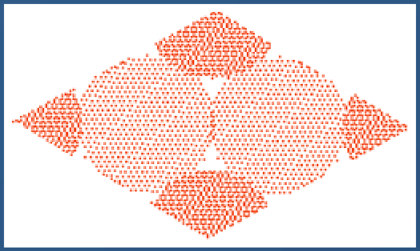


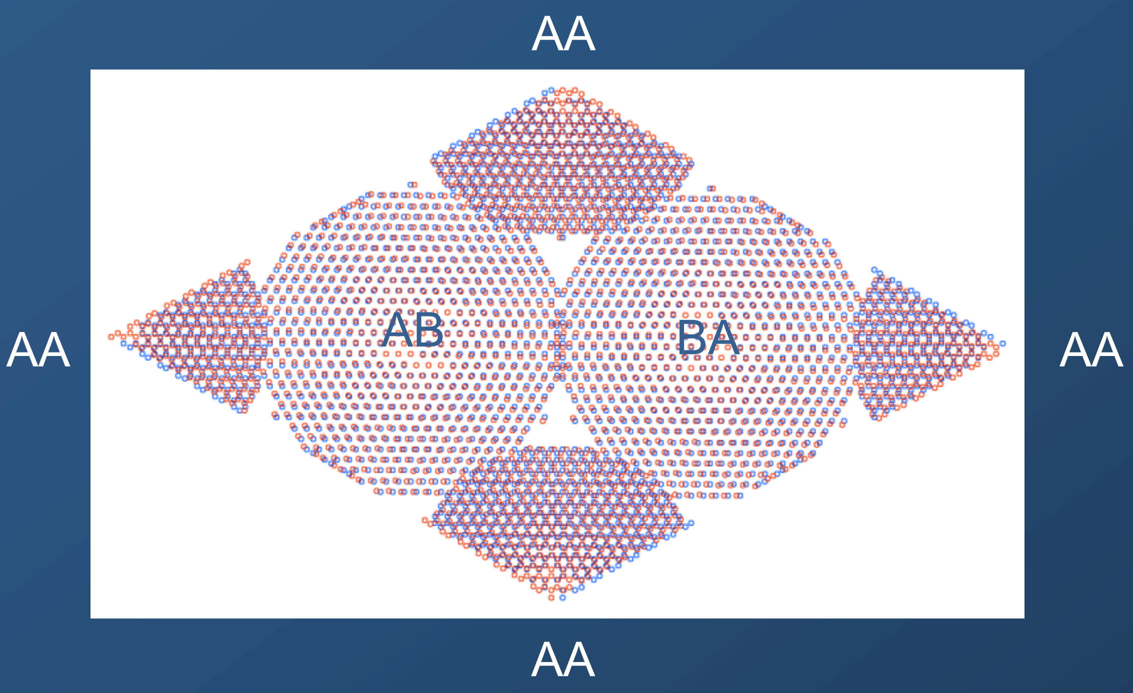
Structure of twisted bilayers



(25,24) $\theta = 1{,}35^{o}$





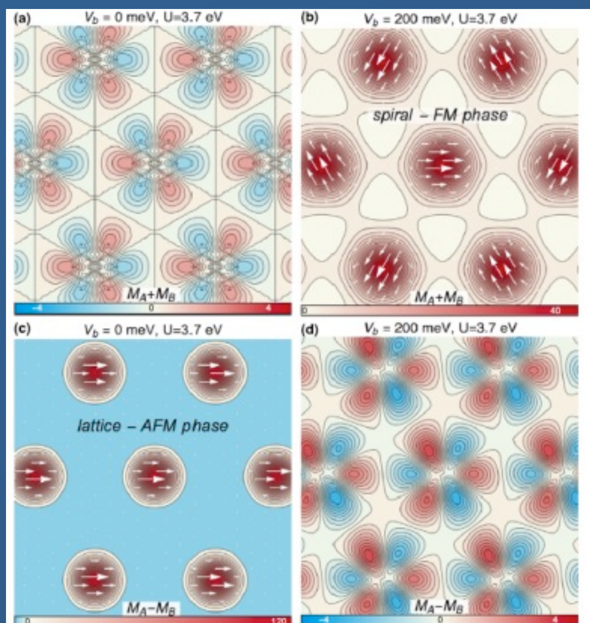


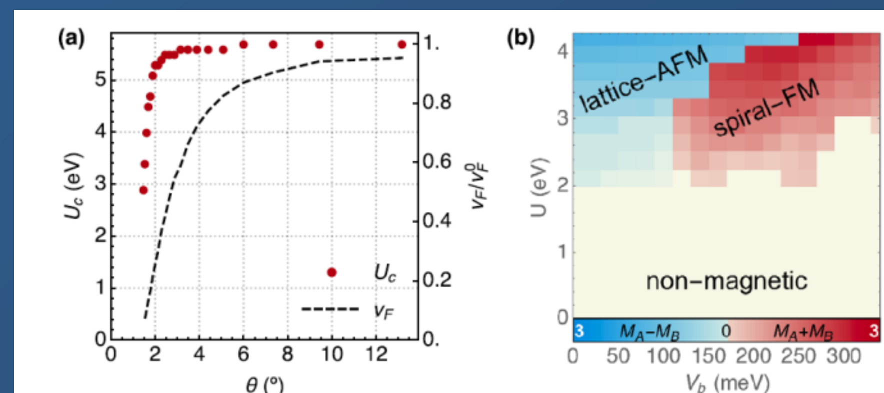
Hubbard interaction

PRL 119, 107201 (2017) PHYSICAL REVIEW LETTERS week ending 8 SEPTEMBER 2017

Electrically Controllable Magnetism in Twisted Bilayer Graphene

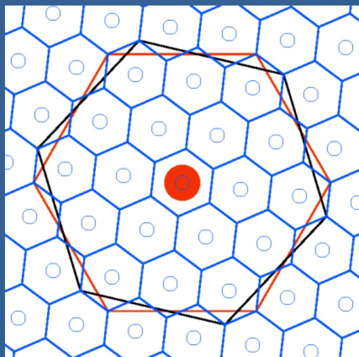
Luis A. Gonzalez-Arraga,[1] J. L. Lado,[2] Francisco Guinea,[1,3] and Pablo San-Jose[4]

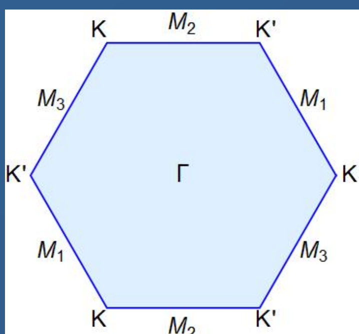




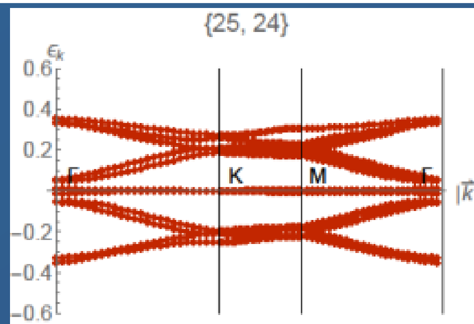
- Mean field theory. Hubbard model. Calculations done in a scaled Moiré unit cell.
- No bias: antiferromagnetism at low values of $\frac{U_c}{t}$
- Finite bias: ferromagnetism due to the existence of flat bands. Antiferromagnetic coupling between neighboring AA regions.

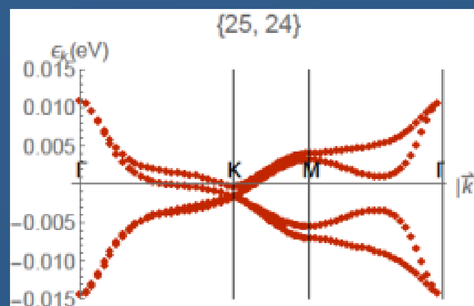
Electronic structure



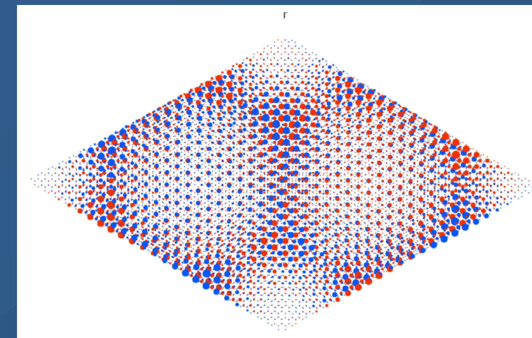


Brillouin zones

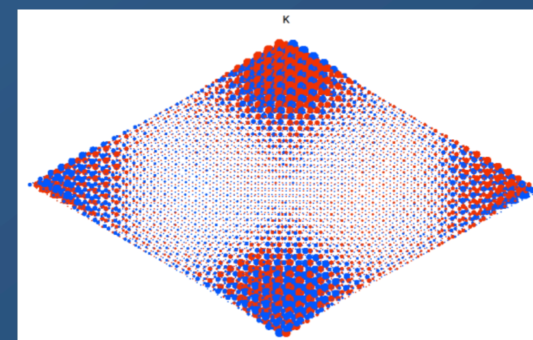




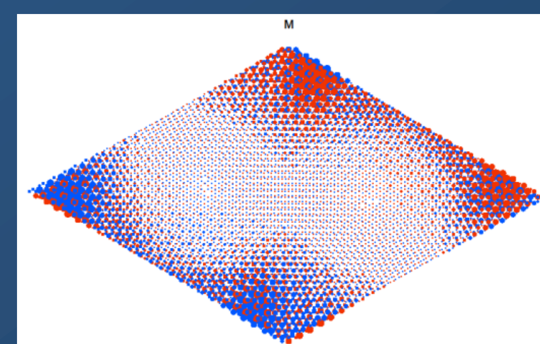
Low energy bands



Γ

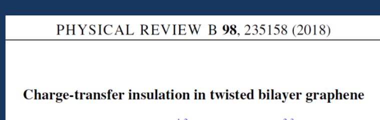


K



M

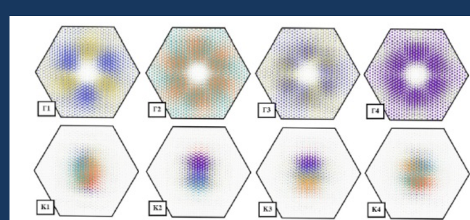
Charge density distribution



PHYSICAL REVIEW B **98**, 235158 (2018)

Charge-transfer insulation in twisted bilayer graphene

Louk Rademaker[1,2] and Paula Mellado[2,3]



Local orbitals and Wannier functions

PHYSICAL REVIEW B 98, 045103 (2018)

Editors' Suggestion

Model for the metal-insulator transition in graphene superlattices and beyond

Noah F. Q. Yuan and Liang Fu

PHYSICAL REVIEW X 8, 031087 (2018)

Maximally Localized Wannier Orbitals and the Extended Hubbard Model for Twisted Bilayer Graphene

Mikito Koshino,[1,*] Noah F. Q. Yuan,[2] Takashi Koretsune,[3] Masayuki Ochi,[1] Kazuhiko Kuroki,[1] and Liang Fu[2]

PHYSICAL REVIEW X 8, 031088 (2018)

Symmetry, Maximally Localized Wannier States, and a Low-Energy Model for Twisted Bilayer Graphene Narrow Bands

Jian Kang[1,*] and Oskar Vafek[1,2,†]

PHYSICAL REVIEW X 8, 031089 (2018)

Origin of Mott Insulating Behavior and Superconductivity in Twisted Bilayer Graphene

Hoi Chun Po,[1] Liujun Zou,[1,2] Ashvin Vishwanath,[1] and T. Senthil[2]

PHYSICAL REVIEW B 98, 085435 (2018)

Editors' Suggestion

Band structure of twisted bilayer graphene: Emergent symmetries, commensurate approximants, and Wannier obstructions

Liujun Zou,[1,2] Hoi Chun Po,[1] Ashvin Vishwanath,[1] and T. Senthil[2]

Electronic bands of twisted graphene layers

1. Model for Metal-Insulator Transition in Graphene Superlattices and Beyond
   Authors: Noah F. Q. Yuan, Liang Fu
   arXiv:1803.09699, Phys. Rev. B 98, 079901 (2018)
2. Origin of Mott Insulating Behavior and Superconductivity in Twisted Bilayer Graphene
   Authors: Hoi Chun Po, Liujun Zou, Ashvin Vishwanath, and T. Senthil
   arXiv:1803.09742, Phys. Rev. X 8, 031089 (2018)
3. Symmetry, Maximally Localized Wannier States, and a Low-Energy Model for Twisted Bilayer Graphene Narrow Bands
   Authors: Jian Kang and Oskar Vafek
   arXiv:1805.04918, Phys. Rev. X 8, 031088 (2018)
4. Maximally-localized Wannier orbitals and the extended Hubbard model for the twisted bilay…
   Authors: Mikito Koshi…
   Kazuhiko Kuroki, Lian…
   arXiv:1805.06819, Phy…
5. Band Structure of T…
   Commensurate App…
   Authors: Liujun Zou, …
   arXiv:1806.07873, Phys. Rev. B 98, 085435 (2018)

Recommended with a Commentary by Francisco Guinea, Imdea

Journal Club for Condensed Matter Physics
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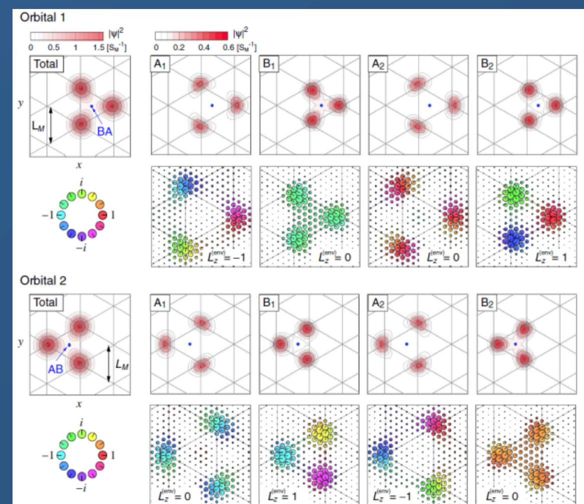
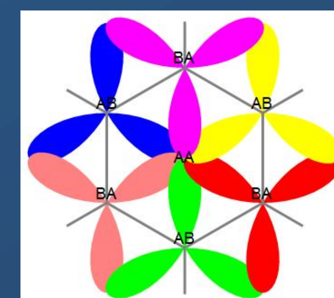
https://www.condmatjclub.org

- The underlying structure of the superlattice is a honeycomb lattice.
- The lattice nodes are at the centers of the regions where the stacking is AB aor BA.
- The Wannier functions have maxima at three lobes around the nodes, and non trivial phases.





This description differs significantly from an array of mesoscopic quantum dots in a triangular lattice.

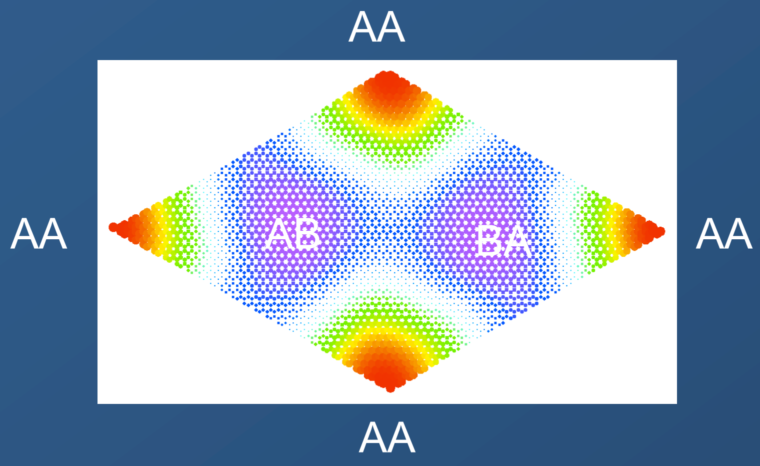
More about interactions

Moiré lattice unit: $\ell_M \approx 15$ nm

Radius of the charge distribution: $\ell_C \approx 5$ nm

Coulomb energy: $E_C \approx \frac{e^2}{\ell_C} \approx 0.1$ eV

On site repulsion: $E_H \approx \frac{U}{N} \approx \frac{U}{(\ell_C/a_0)^2} \approx \frac{e^2 a_0}{\ell_C^2} \approx 0.01$ eV

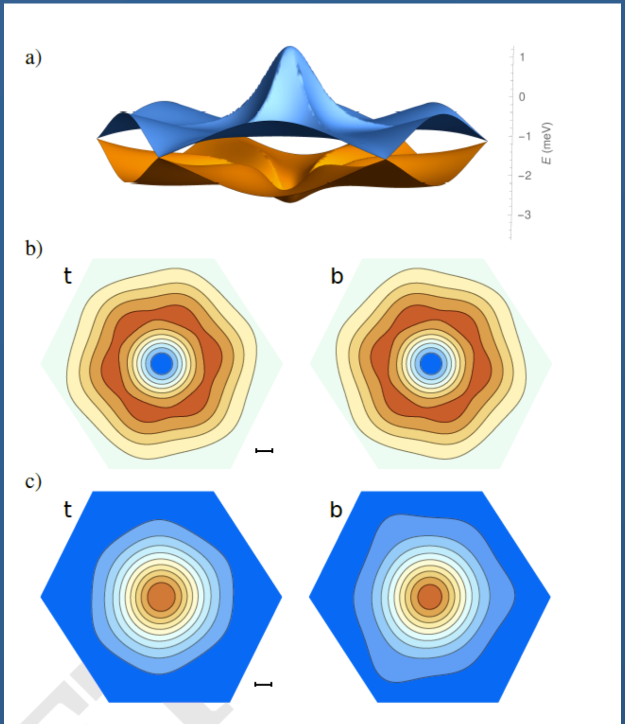


Coulomb potential,

V_{max}=0.029 eV , V_{min}=-0.014eV

Coulomb interactions and screening in twisted graphene bilayers

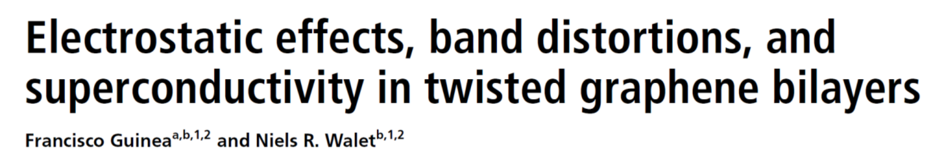
Angle: $\theta = 1.05^o$
Moiré unit cell: $L_M \approx 15\text{nm}$



Γ point

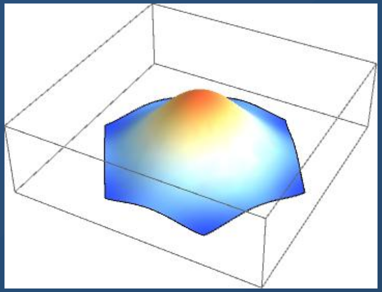
K point

Bands, wavefunctions



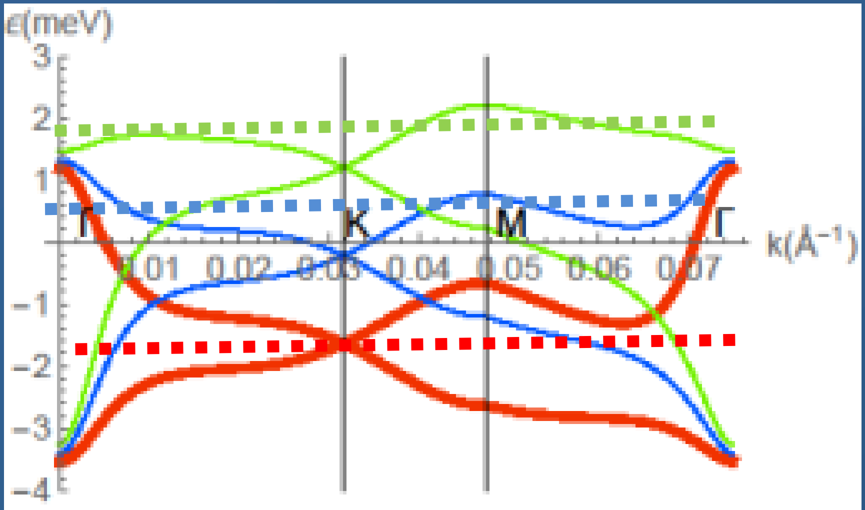
arXiv:1806.05990
Proc. Nat. Acad. Sci. (USA) **115**, 13174 (2019)

- The charge distribution within the Moiré unit cell depends on the state.
- Away from the neutrality point, the charge is concentrated at the center of the unit cell.
- A non uniform electrostatic potential is induced.



Sketch of the electrostatic potential

Twisted bilayers, Hartree approximation



$\Delta V_H = 0$ meV

$\Delta V_H = 5$ meV

$\Delta V_H = 10$ meV

Hartree bands, different fillings.

- The band structure is dependent on filling → new interactions
- The bandwidth increases away from the neutrality point

Exchange term

Renormalization of the Fermi velocity

$$\alpha = \frac{e^2}{\epsilon\hbar v_F} \approx 10^2$$

PHYSICAL REVIEW B VOLUME 59, NUMBER 4 15 JANUARY 1

Marginal-Fermi-liquid behavior from two-dimensional Coulomb interaction

J. González
Instituto de Estructura de la Materia, Consejo Superior de Investigaciones Científicas, Serrano 123, 28006 Madrid, Spain

F. Guinea
Instituto de Ciencia de Materiales, Consejo Superior de Investigaciones Científicas, Cantoblanco, 28049 Madrid, Spain

M. A. H. Vozmediano
Escuela Politécnica Superior, Universidad Carlos III, Butarque 15 Leganés, 28913 Madrid, Spain

$$E_c \frac{d}{dE_c} v_F(E_c) = -\frac{8}{\pi^2} v_F \left(1 + \frac{\arccos g}{g\sqrt{1-g^2}}\right) + \frac{4}{\pi} v_F \frac{1}{g}.$$

nature physics LETTERS
PUBLISHED ONLINE: 24 JULY 2011 | DOI: 10.1038/NPHYS2049

Dirac cones reshaped by interaction effects in suspended graphene

D. C. Elias[1], R. V. Gorbachev[1], A. S. Mayorov[1], S. V. Morozov[2], A. A. Zhukov[3], P. Blake[3], L. A. Ponomarenko[1], I. V. Grigorieva[1], K. S. Novoselov[1], F. Guinea[4]* and A. K. Geim[1,3]

$$\frac{k}{v_F}\frac{\partial v_F}{\partial k} = -\frac{e^2}{4\varepsilon\hbar v_F}$$

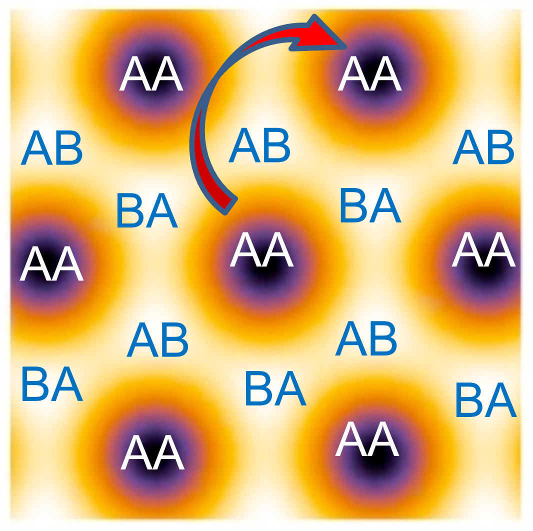
$$\frac{k}{v_F}\frac{\partial v_F}{\partial k} = -\frac{2}{\pi^2}\left[1 - \frac{4\hbar v_F \varepsilon}{N_f e^2} + \frac{8\hbar v_F \arccos\left(\frac{\pi N_f e^2}{8\hbar v_F \varepsilon}\right)}{N_f e^2 \pi \sqrt{1 - \left(\frac{\pi N_f e^2}{8\hbar v_F \varepsilon}\right)^2}}\right]$$

Shift of the occupied Γ point

$$\delta\epsilon_\Gamma^{ex} \approx -\frac{1}{2\pi}\int_0^\Lambda \frac{e^2}{\epsilon k} k\,dk \approx -\frac{e^2\Lambda}{2\pi\epsilon} \approx -0.07\frac{e^2}{\epsilon L_M}$$

The exchange term will increase the bandwidth

New interactions in twisted bilayers



PHYSICAL REVIEW B VOLUME 41, NUMBER 10 1 APRIL 1990

Hole superconductivity and the high-T_c oxides

F. Marsiglio and J. E. Hirsch

41 6435

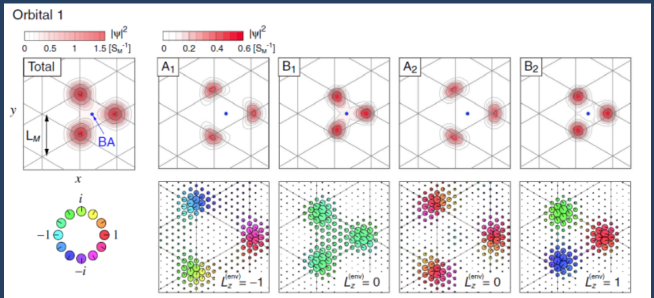
$$\tilde{t}\sum_{i,j}(c_i^\dagger c_j + c_j^\dagger c_i)(n_i + n_j) \qquad \tilde{t} \approx V_H$$

- Electron assisted hopping
- Favorable for superconductivity

PHYSICAL REVIEW X 8, 031087 (2018)

Maximally Localized Wannier Orbitals and the Extended Hubbard Model for Twisted Bilayer Graphene

Mikito Koshino,[1,*] Noah F. Q. Yuan,[2] Takashi Koretsune,[3] Masayuki Ochi,[1] Kazuhiko Kuroki,[1] and Liang Fu[2]



See also

Strong coupling phases of partially filled twisted bilayer graphene narrow bands

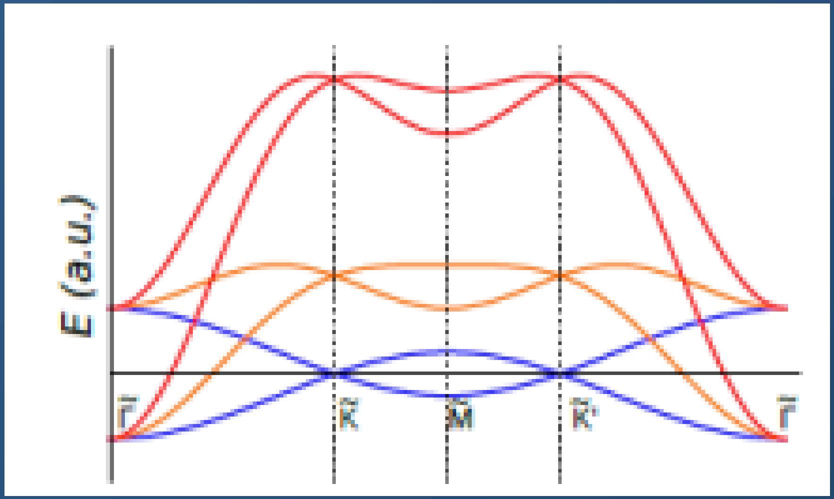
Jian Kang[1,*] and Oskar Vafek[1,2,†]

arXiv:1810.08642

Simple tight binding model

- Description using two orbitals, one at each inequivalent site of the honeycomb lattice.
- Long range hoppings (M. Koshino, N. Yuan, N. Koretsune, K. Kiroki, L. Fu, Phys. Rev. X **8**, 031087 (2018)).
- A simple model for the electrostatic potential describes well the results obtained more sophisticated models.

$$\mathcal{H}_{local} = \mathcal{H}_0 + \mathcal{H}_H = t_1 \sum_{\langle i,j \rangle} c_i^+ c_j + i t_2 \sum_{\langle\langle i,j \rangle\rangle} c_i^+ c_j + V_H \sum_{\langle\langle i,j \rangle\rangle, \{i,j\} \in \{A,B\}} c_i^+ c_j + h.c.$$

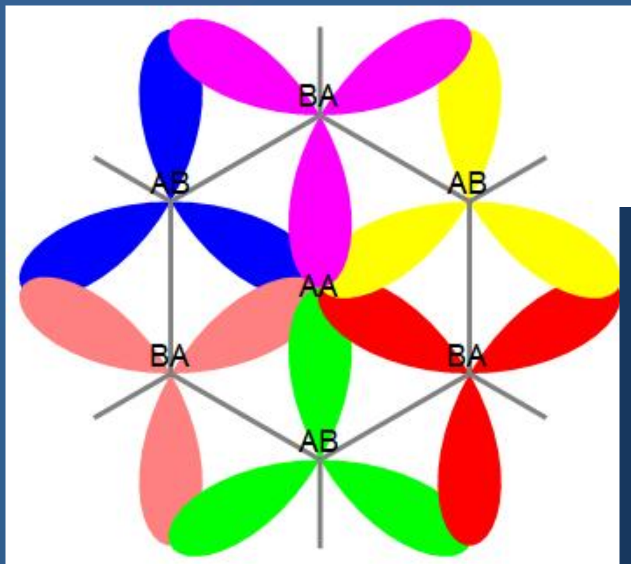


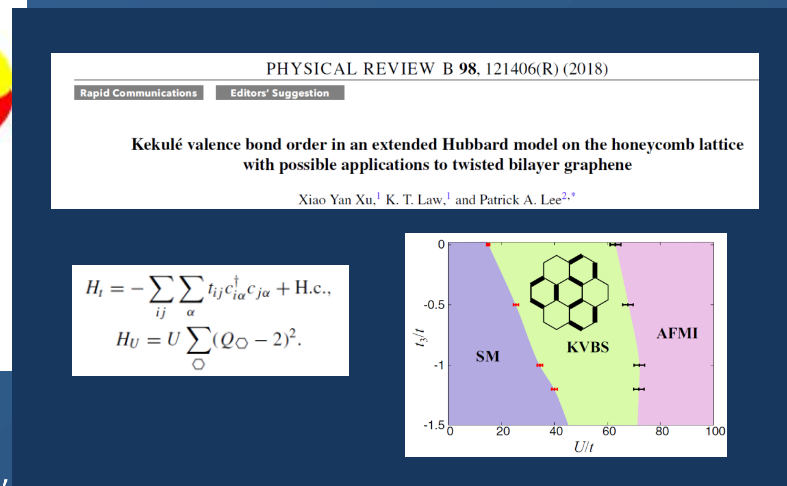
Analysis of the interactions at the Fermi level

$$\mathcal{H}_{int} = \sum_m \left[V_{H_1} \left(\sum_{i=1,\cdots,6} c^+_{i,m} c_{i,m} \right)^2 + V_{H_2} \left(\sum_{i=1,\cdots,6} c^+_{i,m} c_{i,m} \right) \left(\sum_{\langle i,j \rangle} c^+_{i,m} c_{j,m} \right) \right]$$

Local repulsion

Assisted hopping




PHYSICAL REVIEW B **98**, 121406(R) (2018)

Rapid Communications | Editors' Suggestion

Kekulé valence bond order in an extended Hubbard model on the honeycomb lattice with possible applications to twisted bilayer graphene

Xiao Yan Xu,[1] K. T. Law,[1] and Patrick A. Lee[2,*]

$$H_t = -\sum_{ij}\sum_{\alpha} t_{ij} c^{\dagger}_{i\alpha} c_{j\alpha} + \text{H.c.},$$

$$H_U = U \sum_{\hexagon} (Q_{\hexagon} - 2)^2.$$

$\vec{a}_2) + e^{i\vec{k}\prime(\vec{a}_1-\vec{a}_2)}\big)\big] V_{H_1} \sigma_+ \tau_x$

miltonian

$$\Delta_1(\vec{k}) = V_{H_1} \sum_{\vec{k}\prime} f(\vec{k}-\vec{k}') \langle \mathbb{I}_\sigma \tau_x \rangle_{\vec{k}\prime}$$

$$\Delta_2(\vec{k}) = \frac{V_{H_1}}{3} \sum_{\vec{k}\prime} f(\vec{k}-\vec{k}') \left(1 + e^{-i\vec{k}\prime\vec{a}_1} + e^{-i\vec{k}\prime\vec{a}_2}\right) \langle \sigma_- \tau_x \rangle_{\vec{k}\prime}$$

$$\Delta_3(\vec{k}) = \frac{V_{H_1}}{3} \sum_{\vec{k}\prime} f(\vec{k}-\vec{k}') \left(1 + e^{i\vec{k}\prime(\vec{a}_1+\vec{a}_2)} + e^{i\vec{k}\prime(\vec{a}_1-\vec{a}_2)} + e^{i\vec{k}\prime(-\vec{a}_1+\vec{a}_2)}\right) \langle \sigma_- \tau_x \rangle_{\vec{k}\prime}$$

$$\Delta_4(\vec{k}) = V_{H_2} \sum_{\vec{k}\prime} f(\vec{k}-\vec{k}') \left[g(\vec{k}) + g\left(\vec{k'}\right)\right] \langle \mathbb{I}_\sigma \tau_x \rangle_{\vec{k}\prime}$$

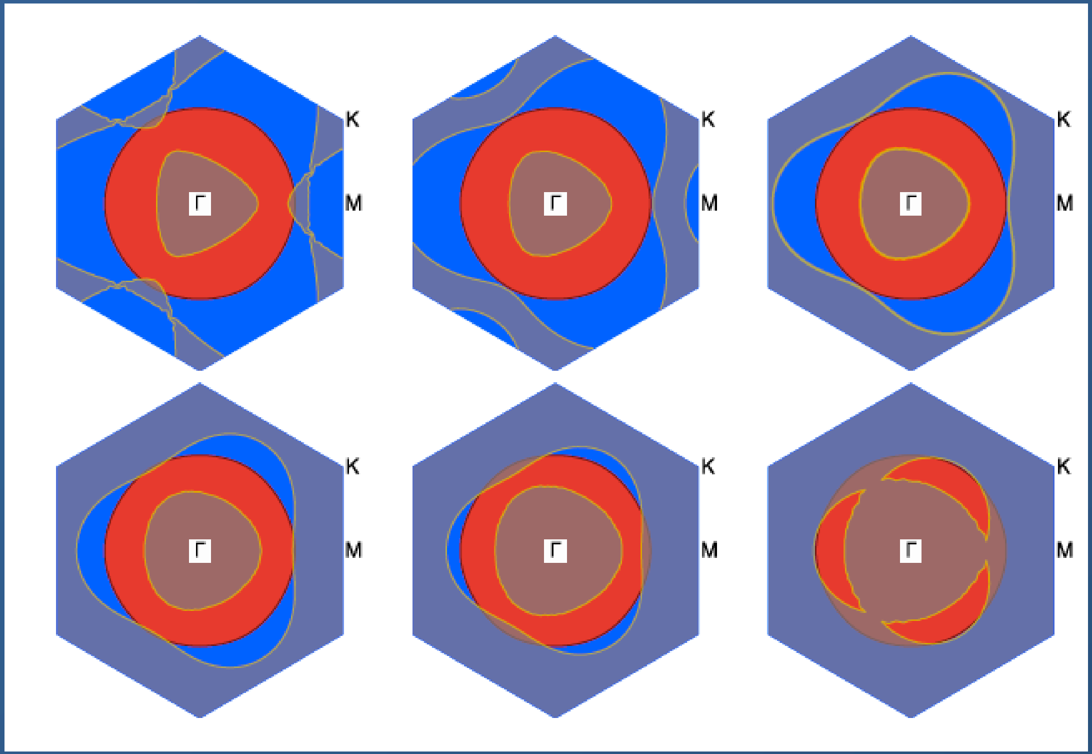
$$\Delta_5(\vec{k}) = V_{H_2} \sum_{\vec{k}\prime} f(\vec{k}-\vec{k}') \left[g(\vec{k}) + g\left(\vec{k'}\right)\right] \langle \sigma_- \tau_x \rangle_{\vec{k}\prime}$$

- Tha gap contains many pieces
- Many superconducting gaps are possible

$$f(\vec{k}) = 3 + 2\cos(k_x) + 4\cos\left(\frac{k_x}{2}\right)\cos\left(\frac{\sqrt{3}k_y}{2}\right)$$

$$g(\vec{k}) = 2\cos(k_x) + 4\cos\left(\frac{k_x}{2}\right)\cos\left(\frac{\sqrt{3}k_y}{2}\right)$$

Superconductivity due to assisted hopping in twisted bilayers



- Example: s-wave superconductivity.
- An attractive interaction appears in some regions of the Brillouin Zone.
- The Fermi surface has two pockets.
- Superconductivity is favored in the blue regions of the Brillouin Zone.

Hartree approximation.
Fermi surfaces for different fillings.

$$T_c \sim W e^{-(W L_M \epsilon)/e^2}$$

Electrostatic interactions and superconductivity

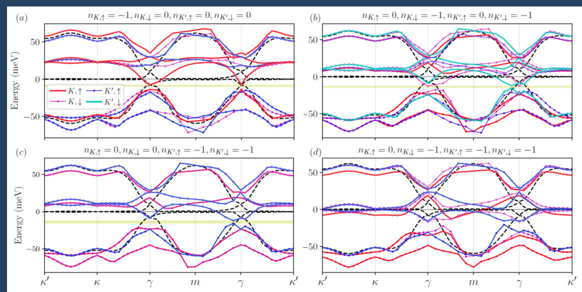
- The low energy electronic states of twisted graphene layers show inhomogeneous charge distributions in the Moiré unit cell.
- Away from the neutrality point, these charge inhomogeneities lead to an electrostatic potential, with a strength comparable or larger than the bandwidth.
  This potential defines the largest interaction between the electrons.
- The electrostatic potential modifies significantly the bands. These deformations can be adscribed to the emergence of new interactions, which can be defined as assisted hopping terms.
- The presence of assisted hopping terms fits naturally with the complex structure of the Wannier functions of the system.
- Assisted hopping is an interaction that favors superconductivty.

Some recent developments

On the Nature of the Correlated Insulator States in Twisted Bilayer Graphene

Ming Xie and A. H. MacDonald

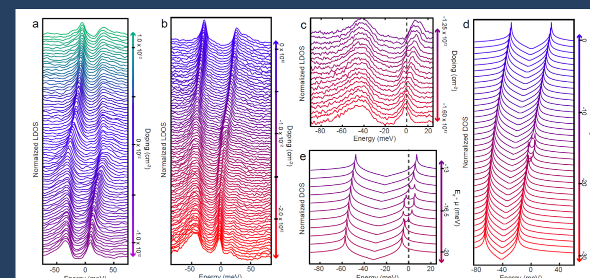
arXiv:1812.04213



Magic Angle Spectroscopy

Alexander Kerelsky,[1] Leo McGilly,[1] Dante M. Kennes,[2] Lede Xian,[3] Matthew Yankowitz,[1] Shaowen Chen,[1,4] K. Watanabe,[5] T. Taniguchi,[5] James Hone,[6] Cory Dean,[1] Angel Rubio,[3,7,*] and Abhay N. Pasupathy[1,†]

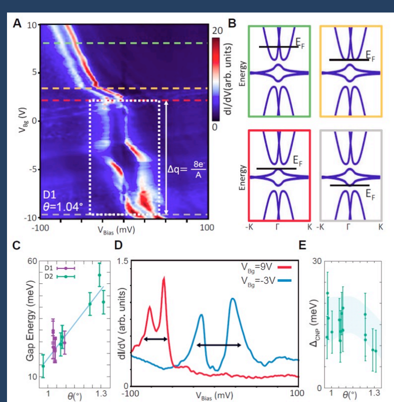
arXiv:1812.08776



Imaging Electronic Correlations in Twisted Bilayer Graphene near the Magic Angle

Youngjoon Choi[1,2,4], Jeannette Kemmer[1,2], Yang Peng [2,3,4], Alex Thomson[2,3,4], Harpreet Arora[1,2], Robert Polski[1,2], Yiran Zhang[1,2,4], Hechen Ren[1,2], Jason Alicea[2,3,4], Gil Refael[2,3,4], Felix von Oppen[2,5], Kenji Watanabe[6], Takashi Taniguchi[6], and Stevan Nadj-Perge[1,2*]

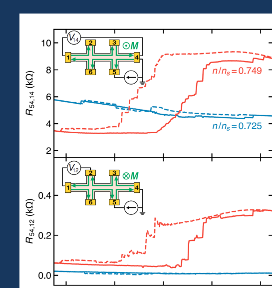
arXiv:1901.02997



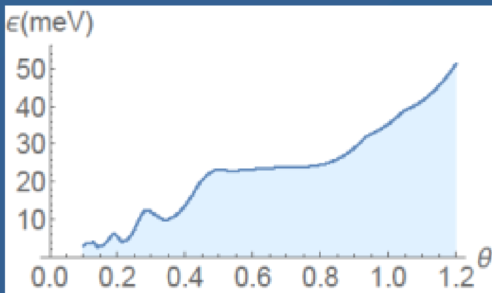
Emergent ferromagnetism near three-quarters filling in twisted bilayer graphene

Aaron L. Sharpe,[1,2*] Eli J. Fox,[2,3*] Arthur W. Barnard,[3] Joe Finney,[3] Kenji Watanabe,[4] Takashi Taniguchi,[4] M. A. Kastner,[3,5,6] David Goldhaber-Gordon[2,3†]

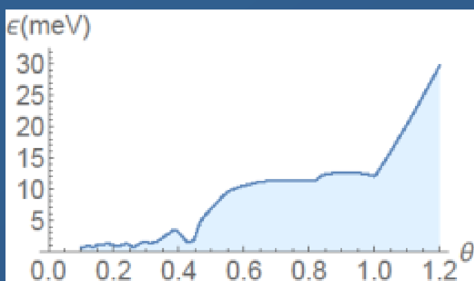
arXiv:1901.03520



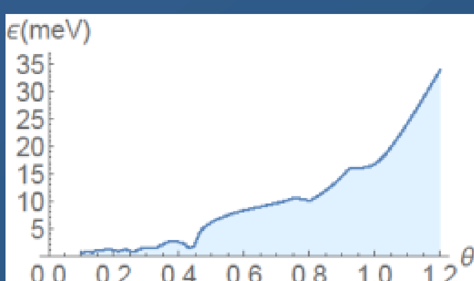
Other narrow band combinations



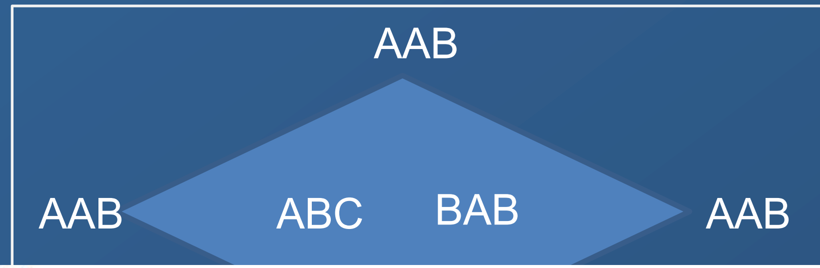
Twisted monolayer on bilayer

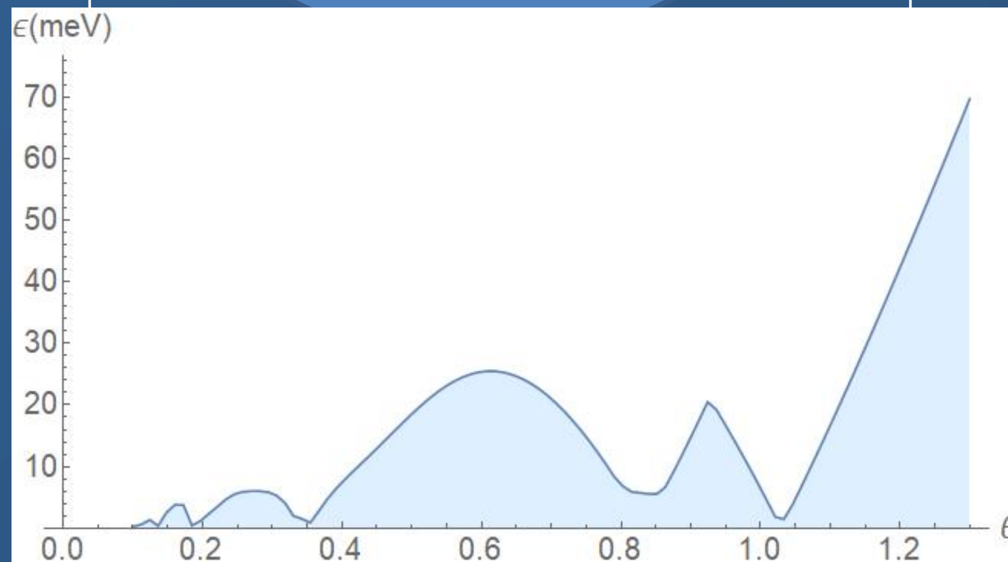


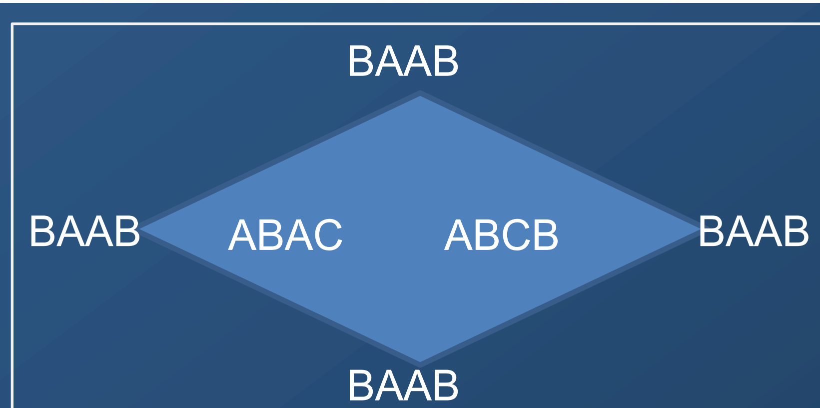
Twisted bilayer on bilayer



Twisted bilayer on bilayer

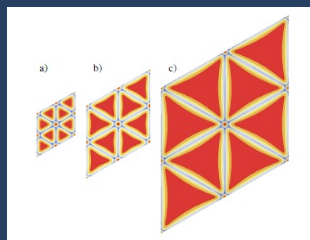






Future work

Strains, lattice relaxation



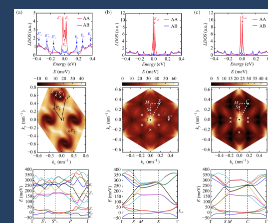
Heterostrains

PHYSICAL REVIEW LETTERS 120, 156405 (2018)

Editors' Suggestion Featured in Physics

Electronic Spectrum of Twisted Graphene Layers under Heterostrain

Loïc Huder,[1] Alexandre Artaud,[1,2] Toai Le Quang,[1] Guy Trambly de Laissardière,[3] Aloysius G. M. Jansen,[1] Gérard Lapertot,[1] Claude Chapelier,[1] and Vincent T. Renard[1]

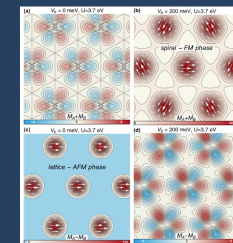


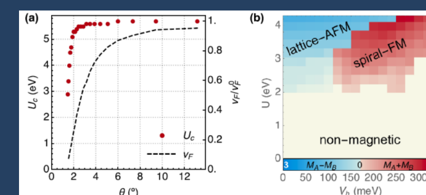
Short range interactions

PRL 119, 107201 (2017) PHYSICAL REVIEW LETTERS week ending 8 SEPTEMBER 2017

Electrically Controllable Magnetism in Twisted Bilayer Graphene

Luis A. Gonzalez-Arraga,[1] J. L. Lado,[2] Francisco Guinea,[1,3] and Pablo San-Jose[4]



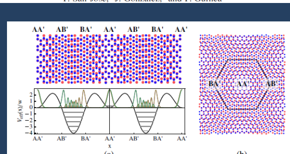


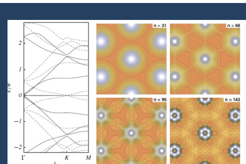
Origin of the magic angles

PRL 108, 216802 (2012) PHYSICAL REVIEW LETTERS week ending 25 MAY 2012

Non-Abelian Gauge Potentials in Graphene Bilayers

P. San-Jose,[1] J. González,[1] and F. Guinea[2]

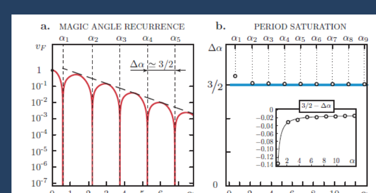




[35] To be precise, while a finite value of $V_{AA'}$ does not destroy subsequent instances of flat-band formation, it does lower their corresponding L as compared to the case $V_{AA'} = 0$, for which they satisfy the simple relation $wL/v_F \approx 2\pi(j + \frac{1}{2})$, for integer j. Moreover, a finite $V_{AA'}$ renders the lowest subband with a small residual bandwidth that is nonexistent in the pure magnetic case.

Origin of Magic Angles in Twisted Bilayer Graphene

Grigory Tarnopolsky, Alex J. Kruchkov, and Ashvin Vishwanath



$$\frac{wL_M}{v_F} \approx 2\pi\left(j + \frac{1}{2}\right)$$

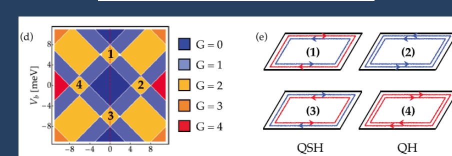
Magnetic and electric fields

2D Materials

PAPER

Quantum spin Hall effect in twisted bilayer graphene

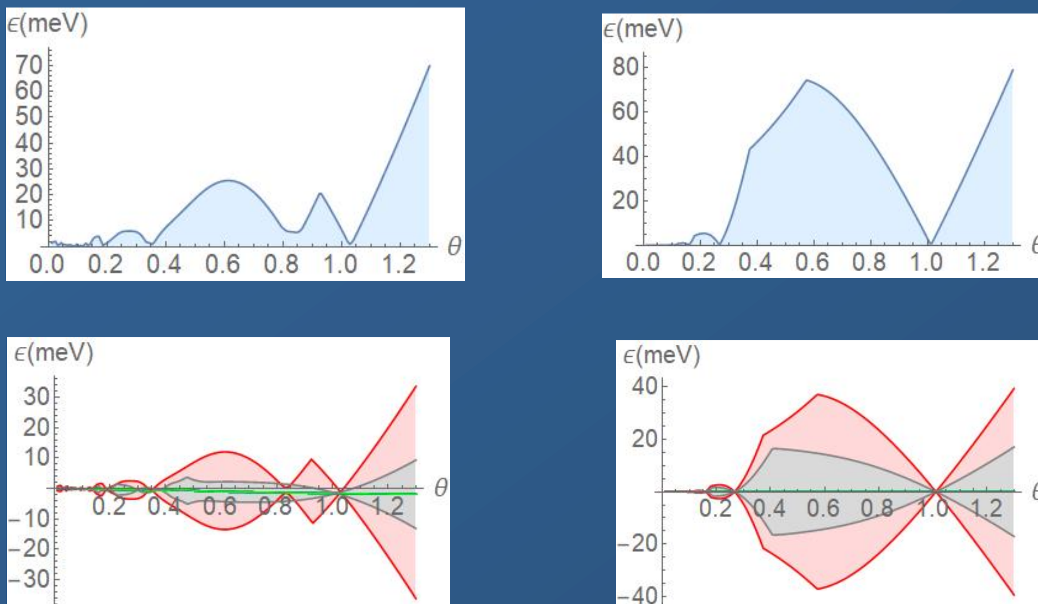
To cite this article: F Finocchiaro *et al* 2017 *2D Mater.* 4 025027



Origin of magic angles

In collaboration with P. San José and J. González

No AA hopping, non Abelian gauge field



$$\mathcal{H} = v_F \vec{\sigma}\left(\mathbb{I}_\tau \vec{\partial} - \vec{A}\right)$$

$$\vec{A} \equiv \left(A_x \tau_x, A_y \tau_y\right)$$

Γ point

M point

K point

$$\frac{w L_M}{v_F} \approx 2\pi\left(j + \frac{1}{2}\right)$$

Multiple topological transitions in twisted bilayer graphene near the first magic angle

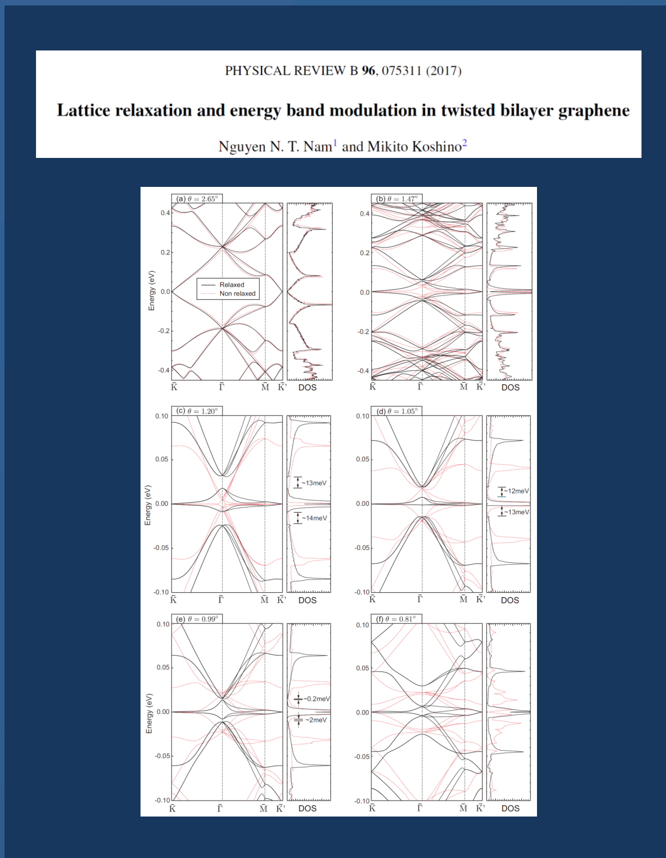
Kasra Hejazi,[1,*] Chunxiao Liu,[1,*] Hassan Shapourian,[2,3] Xiao Chen,[3] and Leon Balents[3]

arXiv:1808.0568

- Magic angles are associated to level crossings.
- Level crossings persist outside high symmetry points.
- Flat bands require non Abelian gauge fields.

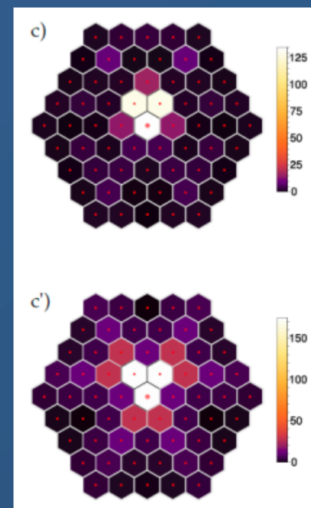
Lattice relaxation, bands

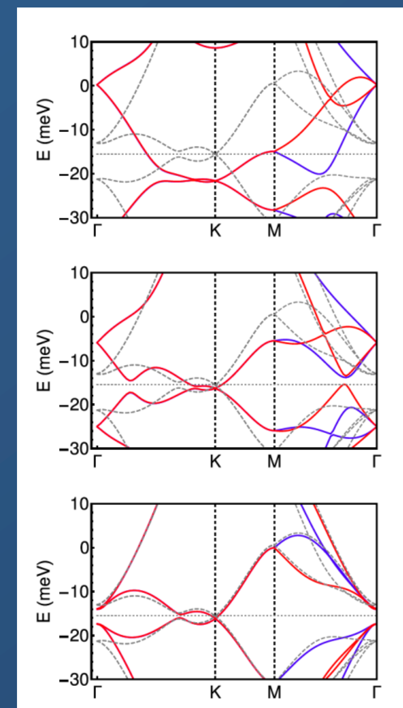
In collaboration with N. Walet


PHYSICAL REVIEW B **96**, 075311 (2017)

Lattice relaxation and energy band modulation in twisted bilayer graphene

Nguyen N. T. Nam[1] and Mikito Koshino[2]





3 harmonics

12 harmonics

48 harmonics

Fully relaxed 32x31 Moiré, $\theta \approx 1.05^o$.
Environment dependent interlayer hoppings.
Comparison between tight binding and continuum models