

Title: Twisted Bilayer Graphene: Moire' is Different

Date: Dec 05, 2018 11:00 AM

URL: <http://pirsa.org/18120017>

Abstract: <p>A single layer graphene hides many body effects in the dense viscous fluid of p - π electrons, Bilayer graphene, with AA and AB registry, on the other hand, exposes some of them. A twisted bilayer springs more surprises. We discuss recently seen superconductivity in twisted bilayer graphene. Resonating valence bond (RVB) physics contained in the dense electron fluid in graphene is invoked [1]. RVB fails to produce superconductivity in neutral graphene, as carrier are absent at the Fermi level. In a twisted bilayer, interlayer tunneling adds equal number of electron and hole carriers in Moire superlattice of dominant AA registry. These carriers use RVB pairing and develop charge $-2e$ and $+2e$ Cooper pair correlations, in spite of Coulomb repulsions. Resulting Moire lattice of Cooper pair puddles form a Josephson lattice. Coulomb blockade makes it a Bosonic Mott insulator. Gate voltage dopes the Bose Mott insulator and interesting consequences follow.</p>

[1] G. Baskaran, arXiv:1804.00627</p>

Twisted Bilayer Graphene **Moire is Different**

4th November 2018



G Baskaran

**PI PERIMETER
INSTITUTE**

Waterloo, Ontario, Canada

Acknowledgement

SERB
Science and Engineering Research Board, DST

Perimeter Institute for Theoretical Physics



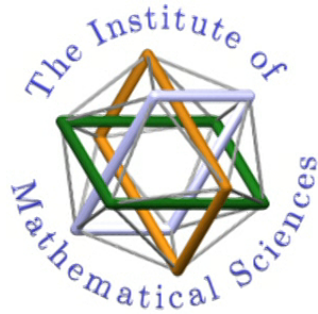
सत्यमेव जयते
Department of
Science & Technology



Waterloo, Ontario
Canada

About my Institute

<http://www.imsc.res.in>



Institute of Mathematical Sciences

Research in

Theoretical Physics
Pure Mathematics
Computer Science

~ 60 faculty
100 Ph.D. students
20 PDF's
10 visitors

Junior Research Fellow

Entrance through **JEST** Exam

Post Doctoral Fellowship

Visiting Research Scholar

Summer Program for BSc, BE, MSc students

Faculty Associateship

Adjunct Faculty

Visiting Professor...

Autonomous Institute

similar to

IIT's

IISc, Bangalore

TIFR, Bombay

Aided by DAE

**MOU exists between Perimeter Institute and
The Institute of Mathematical Sciences**





The Whole is **more than the sum of its parts**
Aristotle

Science, literature, art, .. life ... exemplify this

The **More part differs from situation to situation**

It continues to surprise us & makes **emergence exciting ...**

4 August 1972, Volume 177, Number 4047

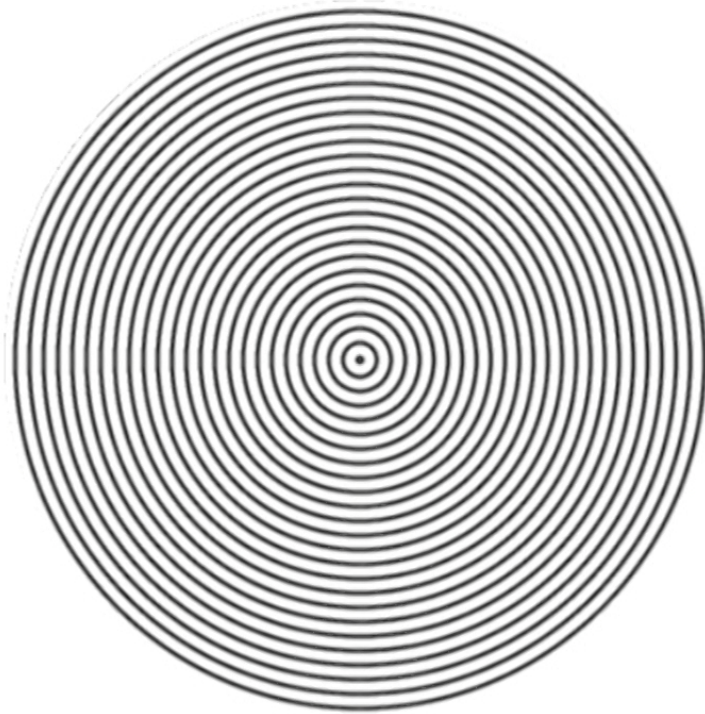
SCIENCE

More Is Different

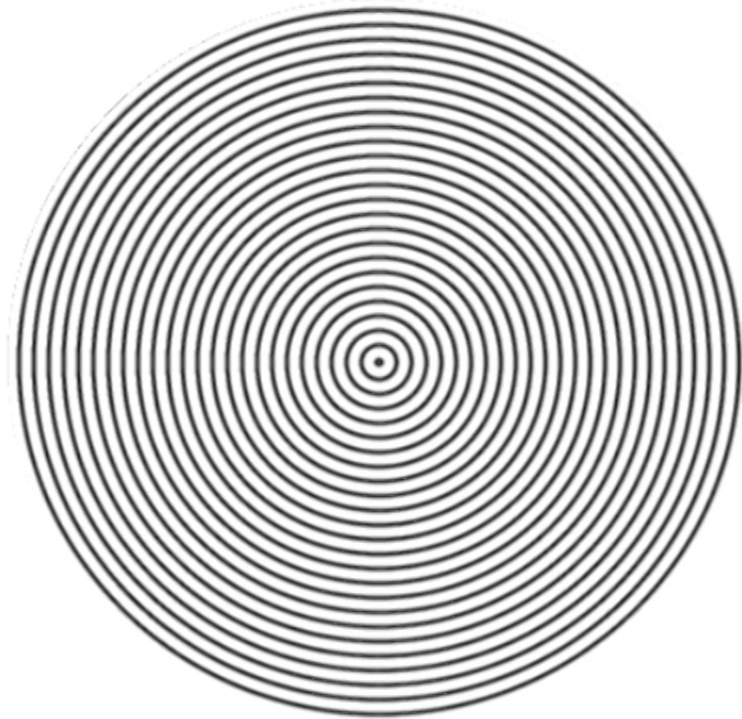
Broken symmetry and the nature of
the hierarchical structure of science.

P. W. Anderson





A

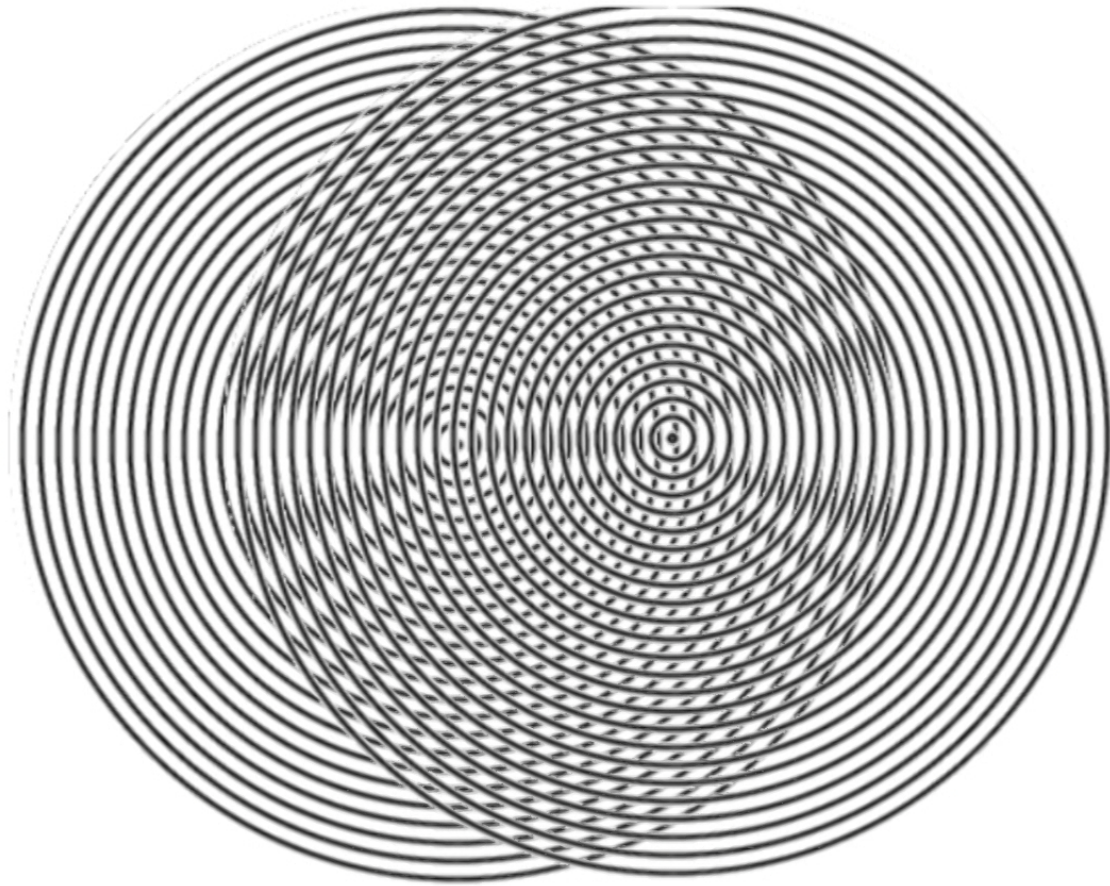


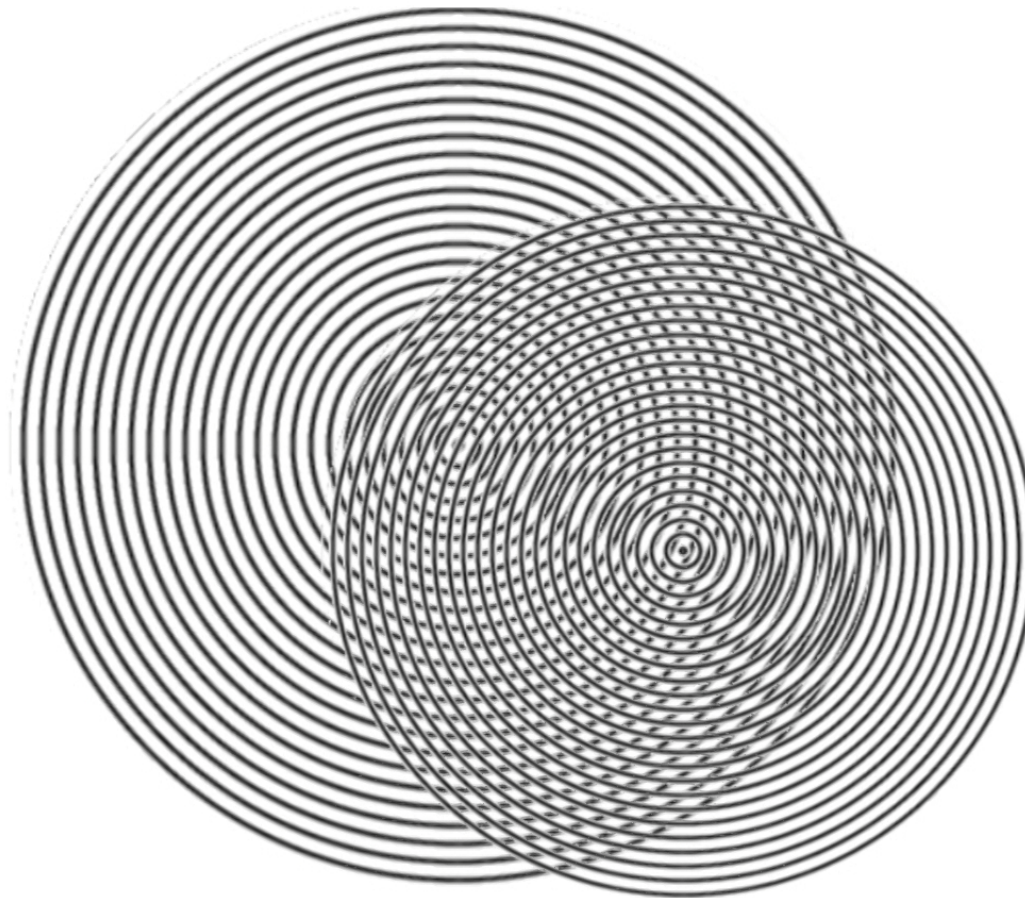
A

Complexity and Emergence

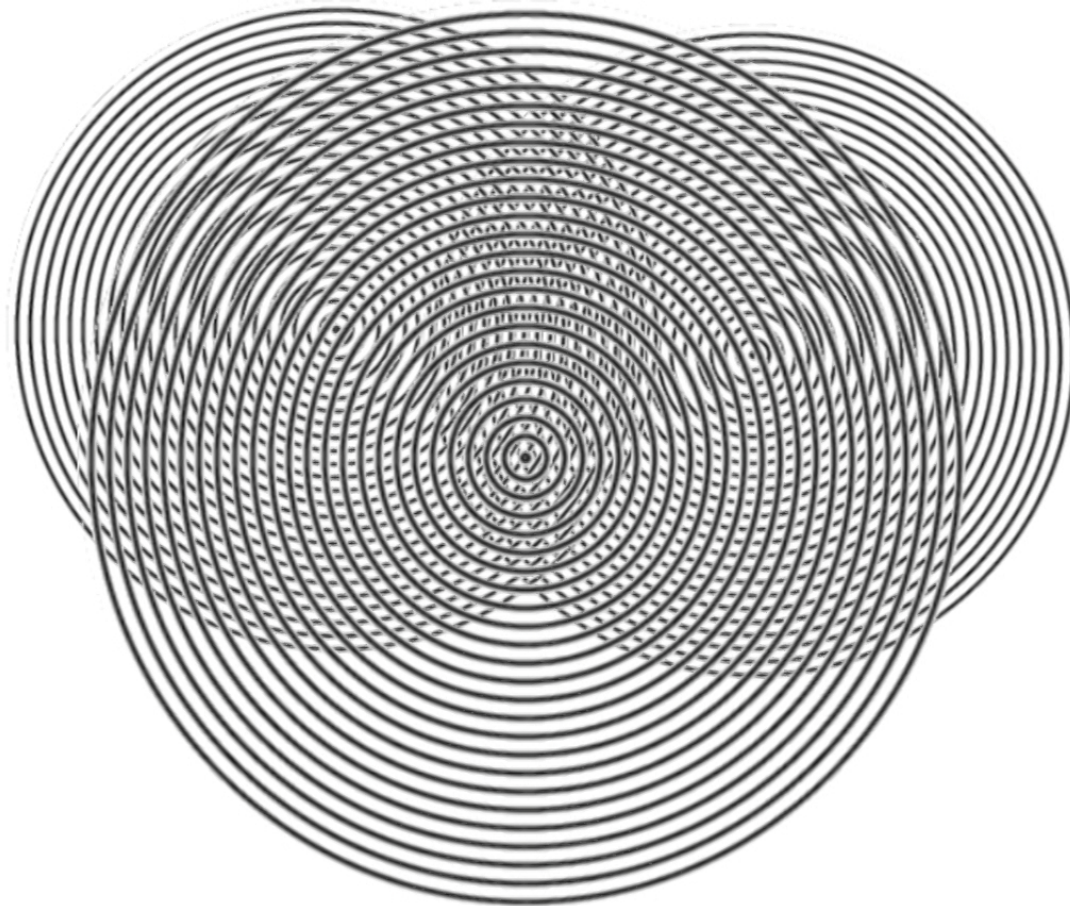
More Than the Sum of the Parts

$$A + A > 2A$$





Moire patterns

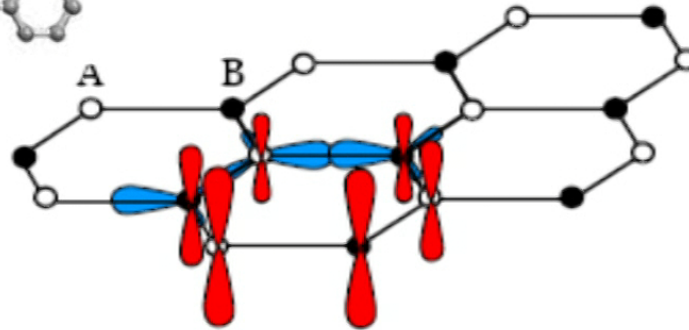
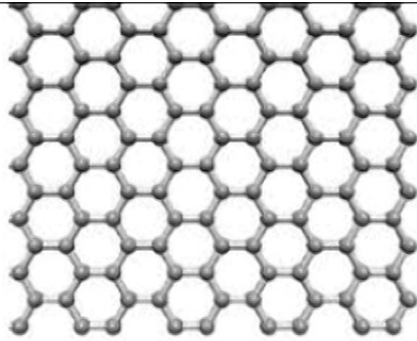




Kavin



19th April 2018



- σ - bonds in the xy-plane: sp^2 hybridization of the $2s$, $2p_x$ and $2p_y$ orbitals
- π - bonds the fourth valence electron ($2p_z$ orbitals) is in a π -orbital with its lobes perpendicular to the plane

Transport properties of graphene are determined by the delocalized π electrons (one per C atom)

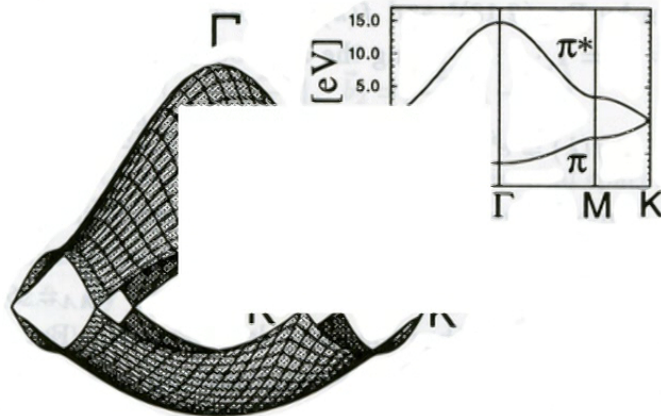
Band structure

- **Tight-binding model; nearest-neighbor interaction**

Wallace, PR 71,622 (1947)

$$E(k_x, k_y) = \pm t \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_y a}{2}\right) \cos\left(\frac{k_x a}{2}\right) + 4 \cos^2\left(\frac{k_x a}{2}\right)}$$

$t \approx 2.5$ eV overlap integral between nearest neighbors



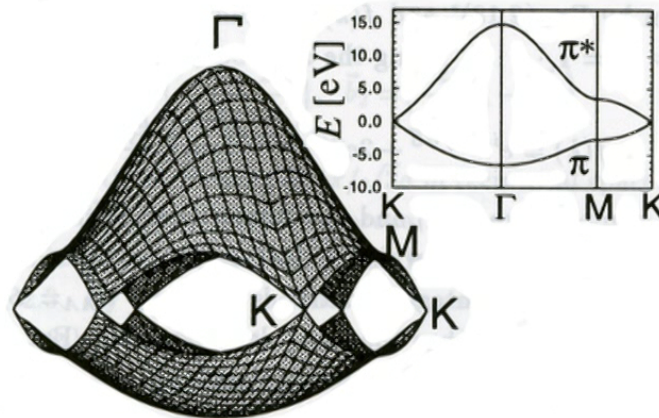
Band structure

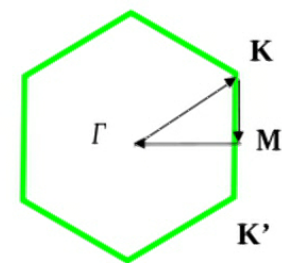
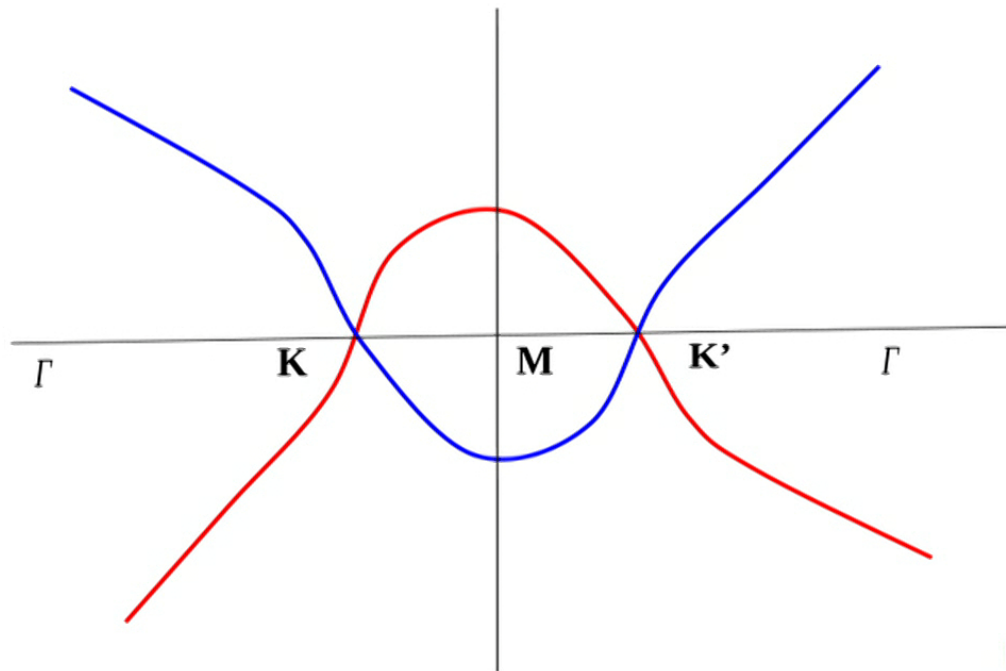
- **Tight-binding model; nearest-neighbor interaction**

Wallace, PR 71,622 (1947)

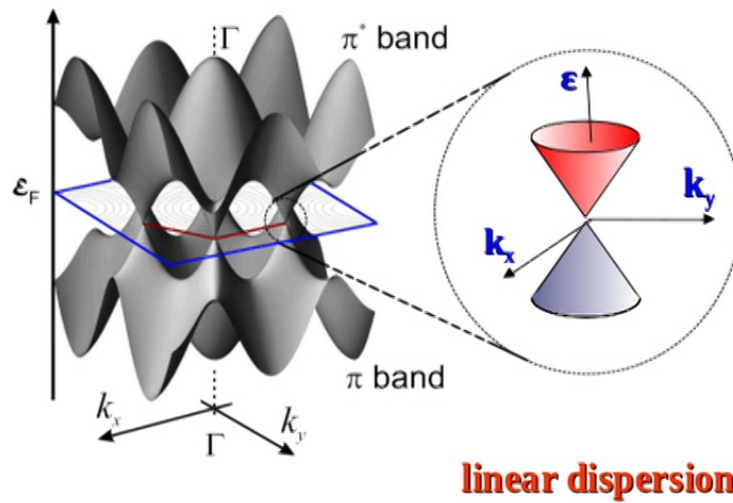
$$E(k_x, k_y) = \pm t \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_y a}{2}\right) \cos\left(\frac{k_x a}{2}\right) + 4 \cos^2\left(\frac{k_x a}{2}\right)}$$

$t \approx 2.5$ eV overlap integral between nearest neighbors

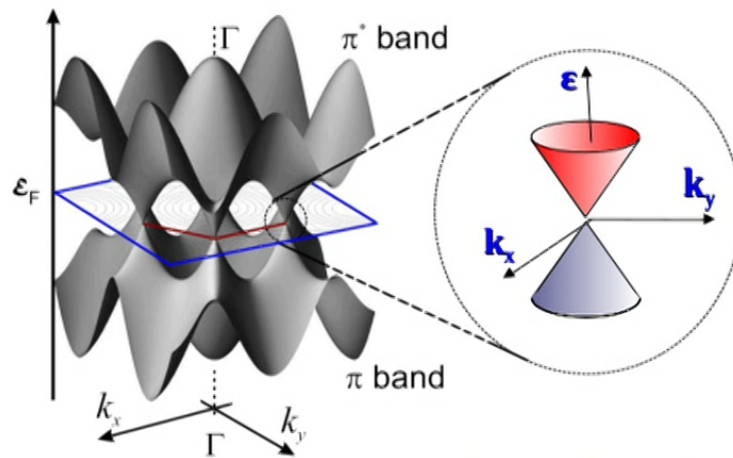




Near the K (K') points

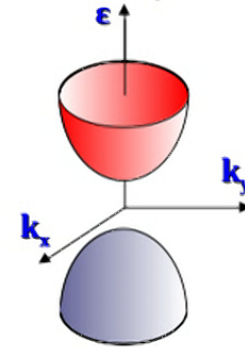


Near the K (K') points



linear dispersion

Conventional 2D electron system

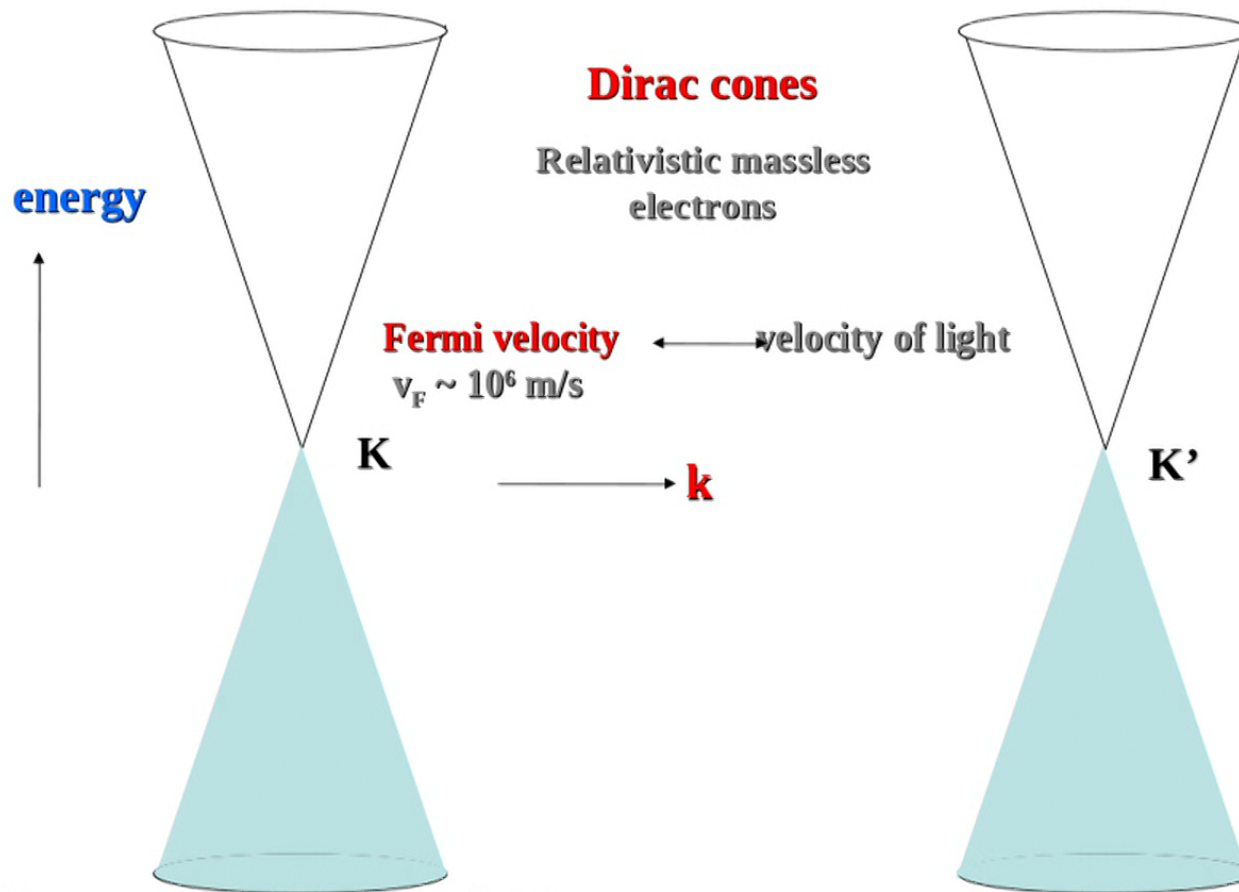


quadratic dispersion

- In the vicinity of the K (K') points:

$$\varepsilon(\mathbf{k}) = \pm \left(\frac{3ta_{c-c}}{2} \right) |\mathbf{k}| = \pm \hbar v_F |\mathbf{k}|$$

- \mathbf{k} is measured with respect to the K (K') point
- $v_F \sim 10^6$ m/s \rightarrow Fermi velocity



This approximation is very helpful to do calculation analytically and gain good physical insight

**Parity anomaly (Semenoff, Haldane 1983)
spin Hall effect eg. Kane, Mele, PRL 2004**

Massless Dirac fermions

- **Unique band structure just described brings profound changes in the electronic properties of the system**
- **Effective-mass approximation: The Hamiltonian near the K point is**

$$H_{\mathbf{K}}(\mathbf{k}) = \frac{3ta_{c-c}}{2} \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} = \hbar v_F \boldsymbol{\sigma} \cdot \mathbf{k}$$

where $\boldsymbol{\sigma}$ are the 2×2 Pauli matrices

- **Near the K' point:**

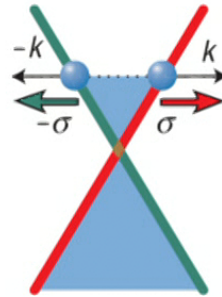
$$H_{\mathbf{K}'}(\mathbf{k}) = - \hbar v_F \boldsymbol{\sigma}^* \cdot \mathbf{k}$$

- **The Schrödinger equation then transforms into a relativistic Dirac equation with vanishing rest mass**

Dirac Weyl Fermions in condensed matter !

Massless Chiral fermions

- The upper and lower components correspond to the quantum-mechanical amplitudes (or 'pseudospin') of finding the particle on one of the two sublattices
- Graphene: 'pseudospin' direction is linked with the 'momentum' of the particles

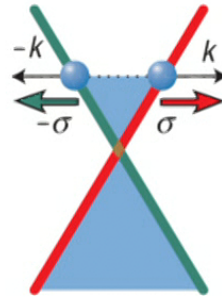


⇒ wavefunctions in the vicinity of K and K' point are 'chiral' (helical fermions) (Geim et al.)

⇒ scattering of particles from k to $-k$ (backscattering) is suppressed (Ando et al.)

Massless Chiral fermions

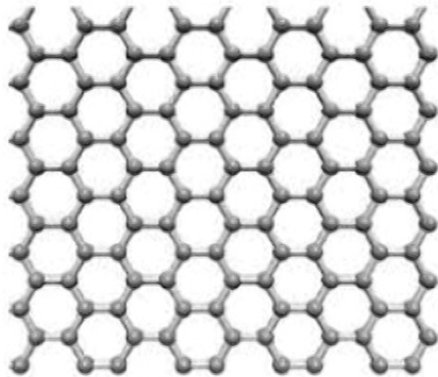
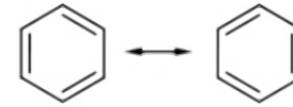
- The upper and lower components correspond to the quantum-mechanical amplitudes (or 'pseudospin') of finding the particle on one of the two sublattices
- **Graphene: 'pseudospin' direction is linked with the 'momentum' of the particles**



⇒ wavefunctions in the vicinity of K and K' point are 'chiral' (helical fermions) (Geim et al.)

⇒ scattering of particles from k to $-k$ (backscattering) is suppressed (Ando et al.)

- **Particles have opposite chirality in the K and K' valleys or in the electron or hole bands**



At low energy scales graphene behaves as a Fermi liquid or a Dirac liquid

However, Preformed Cooper pairs or Singlet pairing exist **Off shell**

This is related to Paulings Resonating Valence Bond Correlations

Graphene is a Sleeping Superconductor

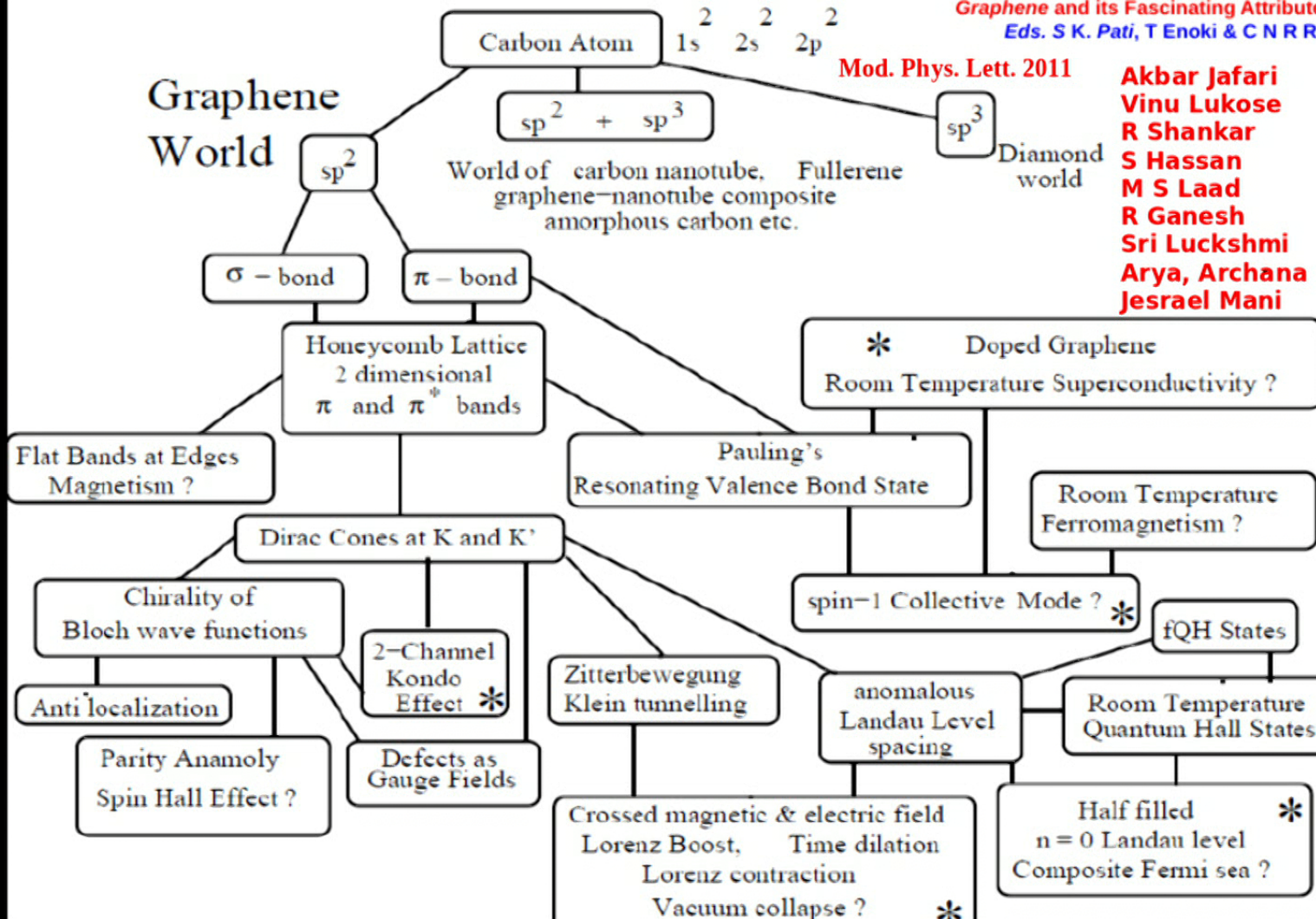
Quantum Complexity in Graphene

G Baskara

Graphene and its Fascinating Attributes
Eds. S K. Pati, T Enoki & C N R Rao

Mod. Phys. Lett. 2011

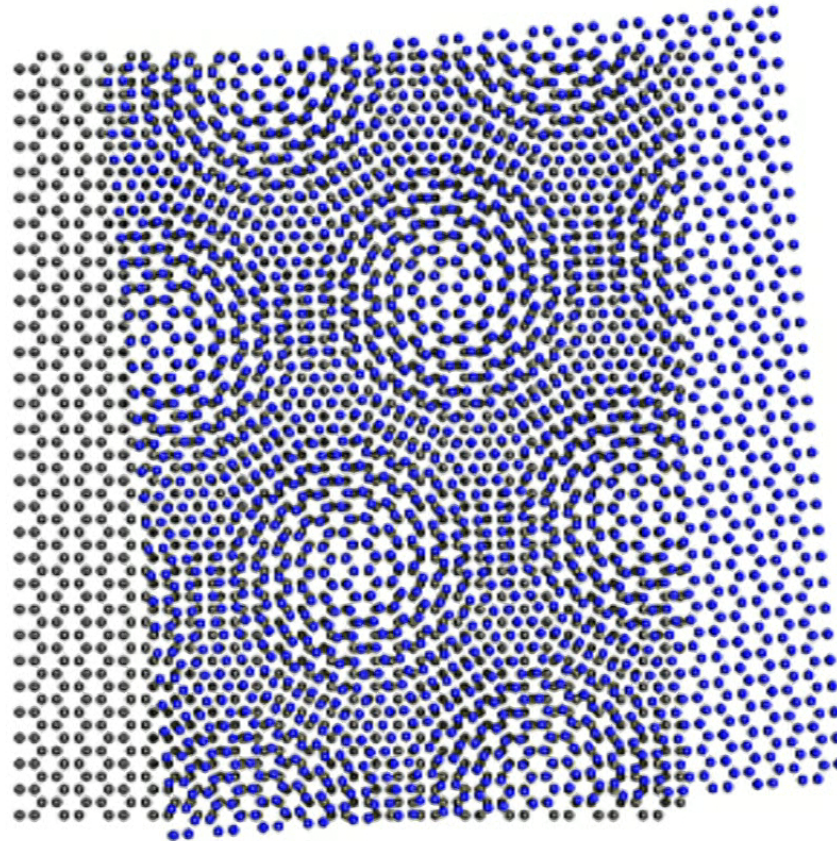
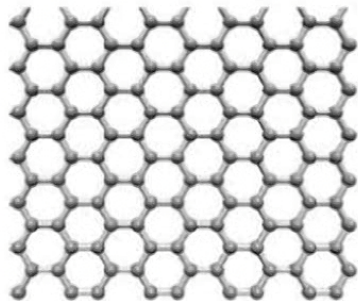
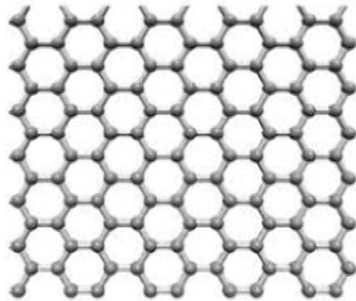
Akbar Jafari
Vinu Lukose
R Shankar
S Hassan
M S Laad
R Ganesh
Sri Luckshmi
Arya, Archana
Jesrael Mani



Unconventional superconductivity in magic-angle graphene superlattices

Yuan Cao¹, Valla Fatemi¹, Shiang Fang², Kenji Watanabe³, Takashi Taniguchi³, Efthimios Kaxiras^{2,4} & Pablo Jarillo-Herrero¹

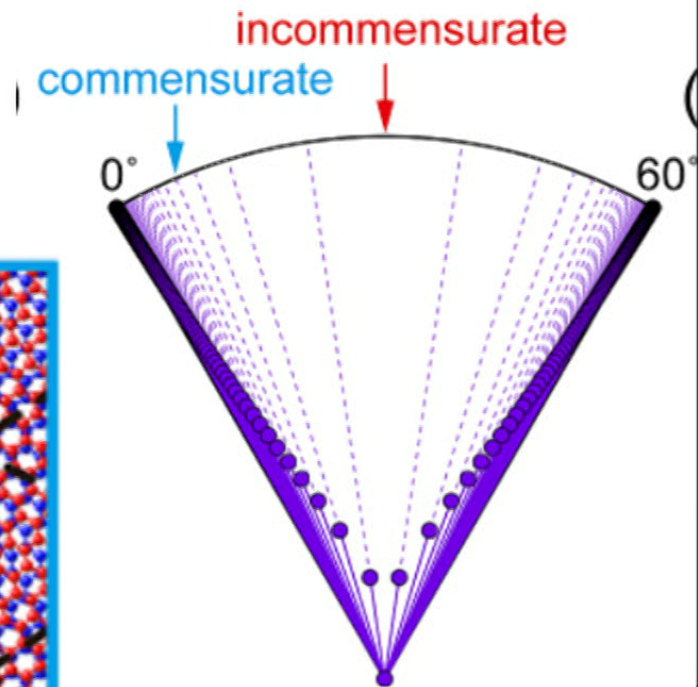
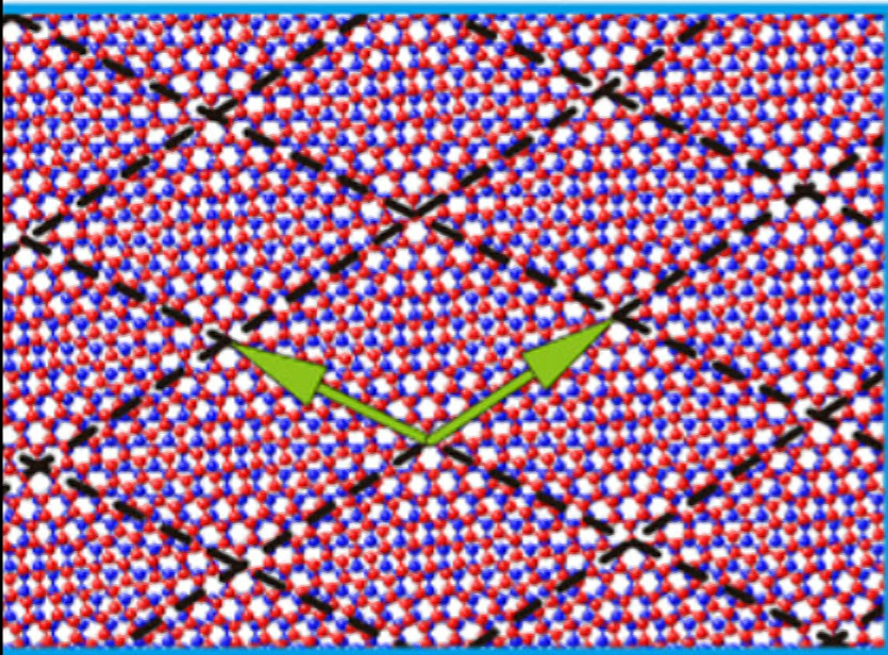
1. Cao, Y. *et al. Nature* <http://dx.doi.org/10.1038/nature26160> (2018).
2. Cao, Y. *et al. Nature* <http://dx.doi.org/10.1038/nature26154> (2018).

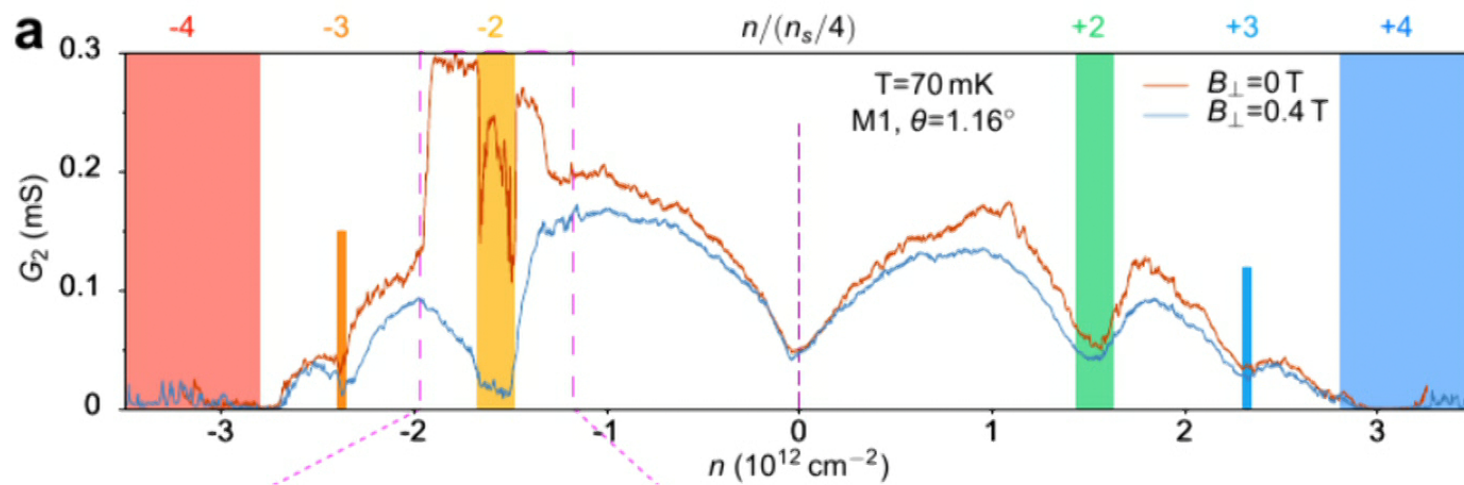
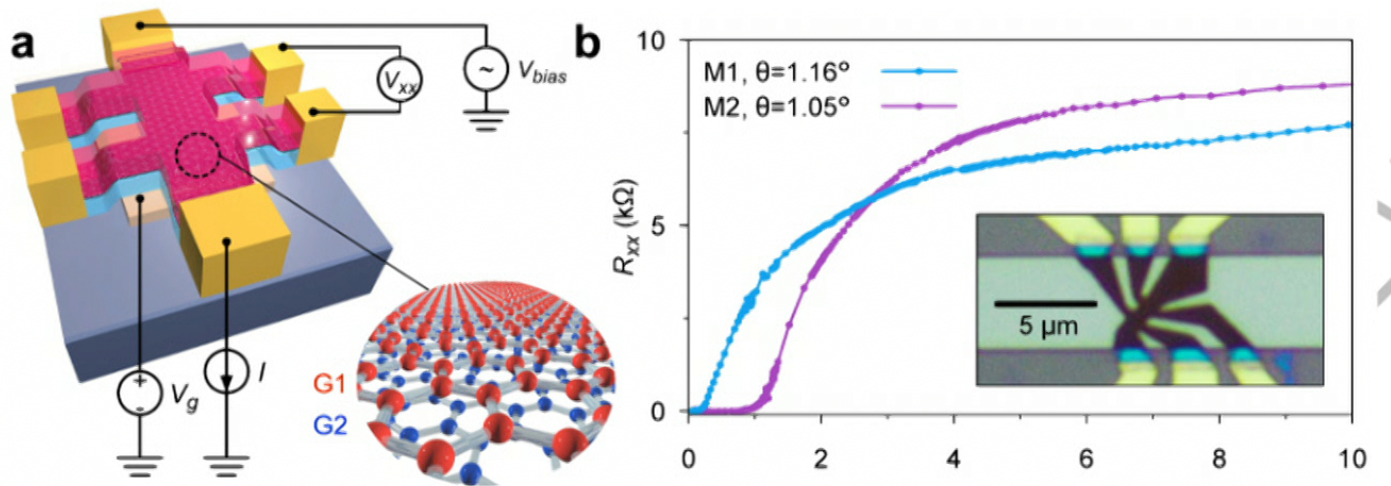


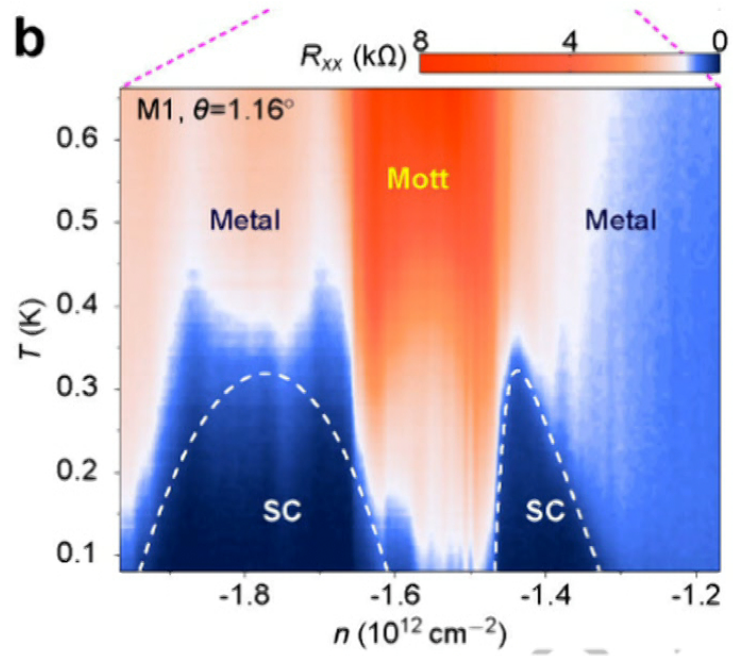
Yao et al.,

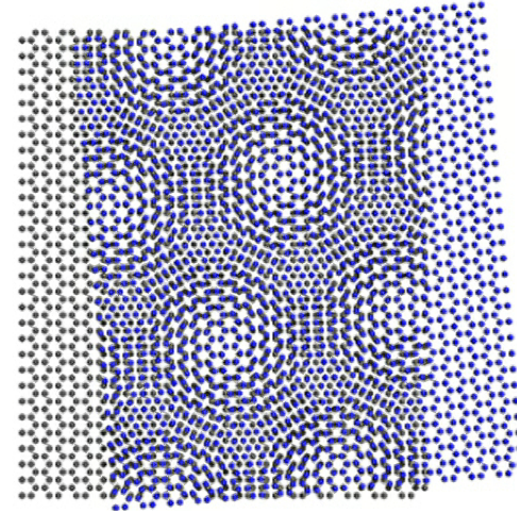
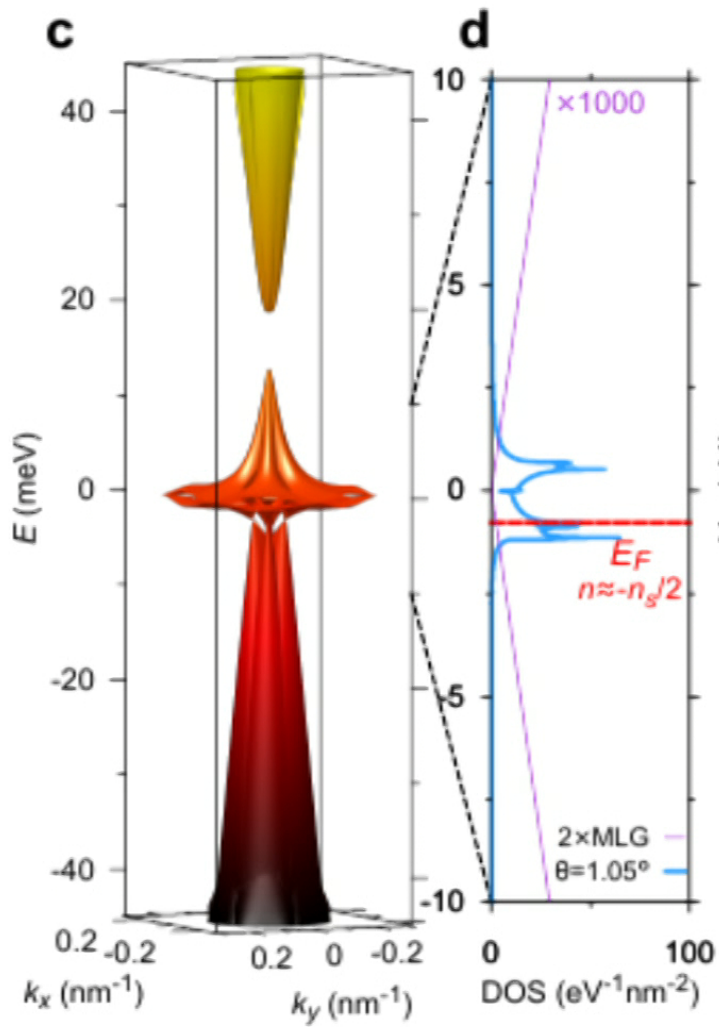
arXiv:1804.05372

commensurate superlattice





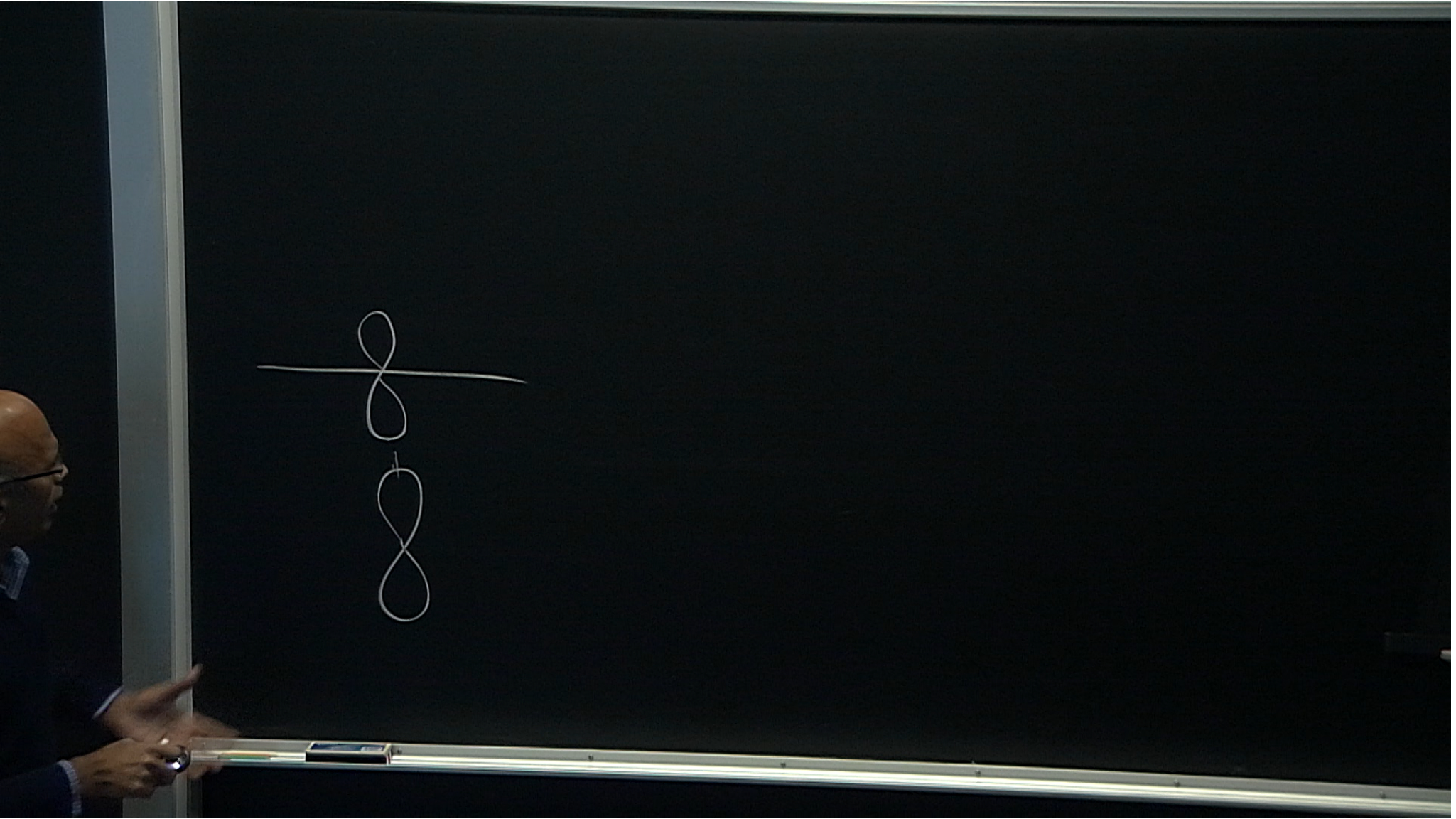




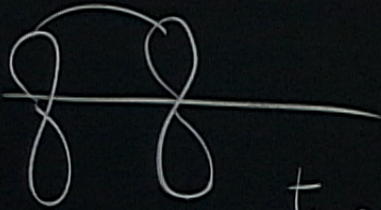
At the magic angle of 1.16 degree
 number of carbon atoms
 per unit cell is about 2000

What happens when we put two graphene layers on top of each other ?

- They communicate via quantum mechanical hopping of electrons between top and bottom 2pz orbitals of C atom that are close to each other
- Interlayer hopping matrix element is ~ 0.3 eV
(this is small compared to in plane hopping ~ 3 eV)
- To gain delocalization or tunneling energy carbon atoms of graphene lattices will also relax
- Bloch states of electrons will get modified
- Are there interesting manybody effects ?



$t \sim 3\text{eV}$

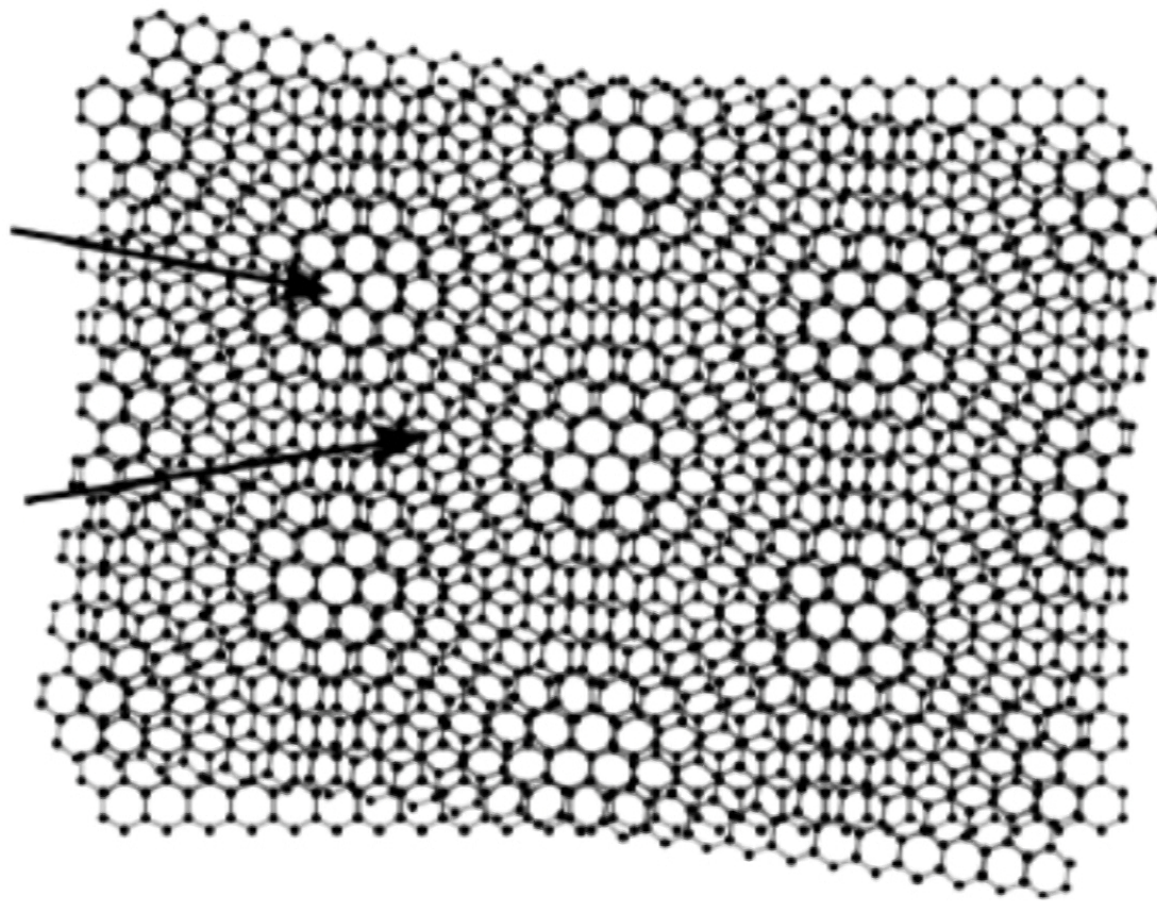


$t_{\perp} \sim 0.3$

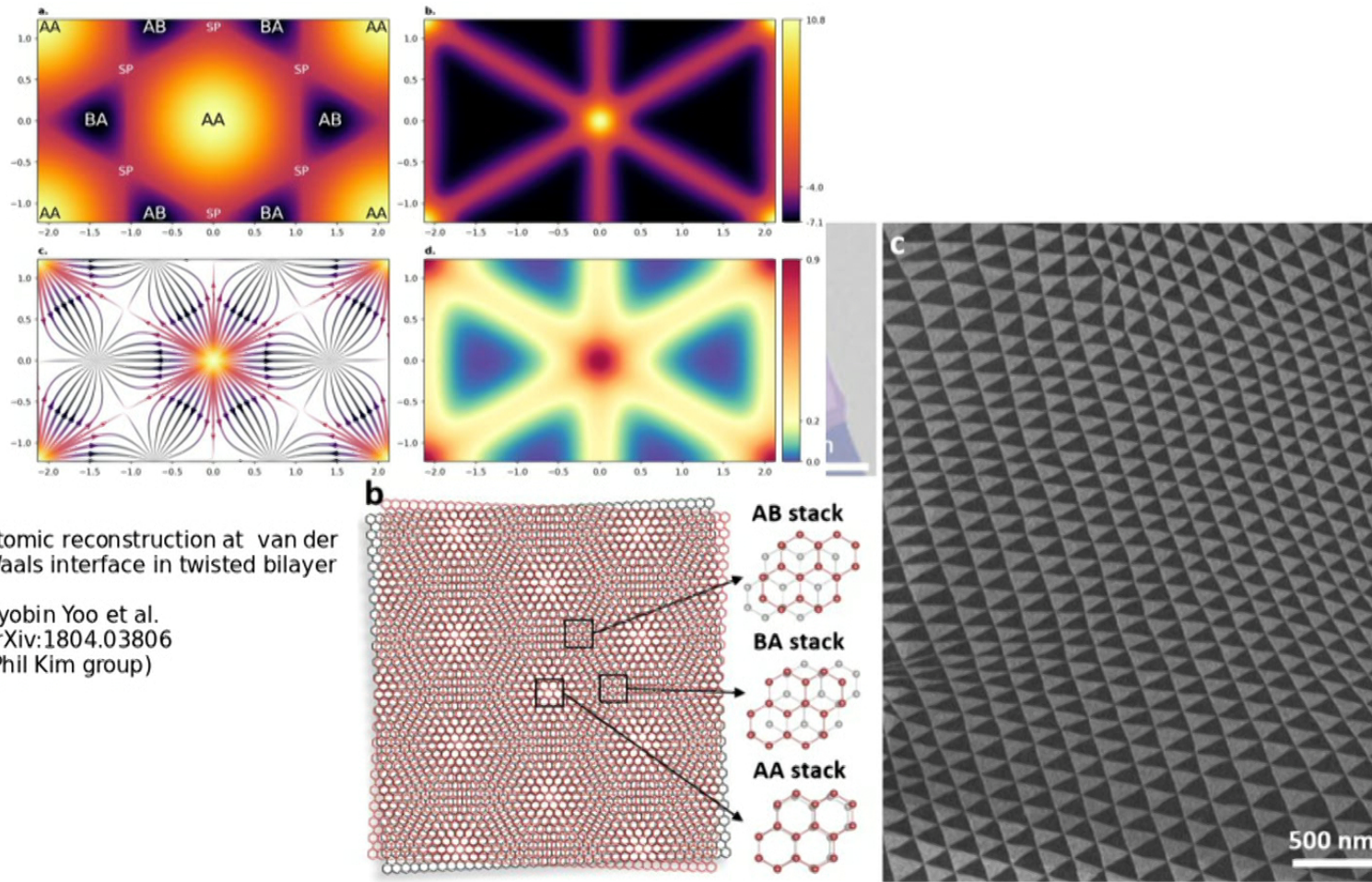


AA
stacking

AB
stacking

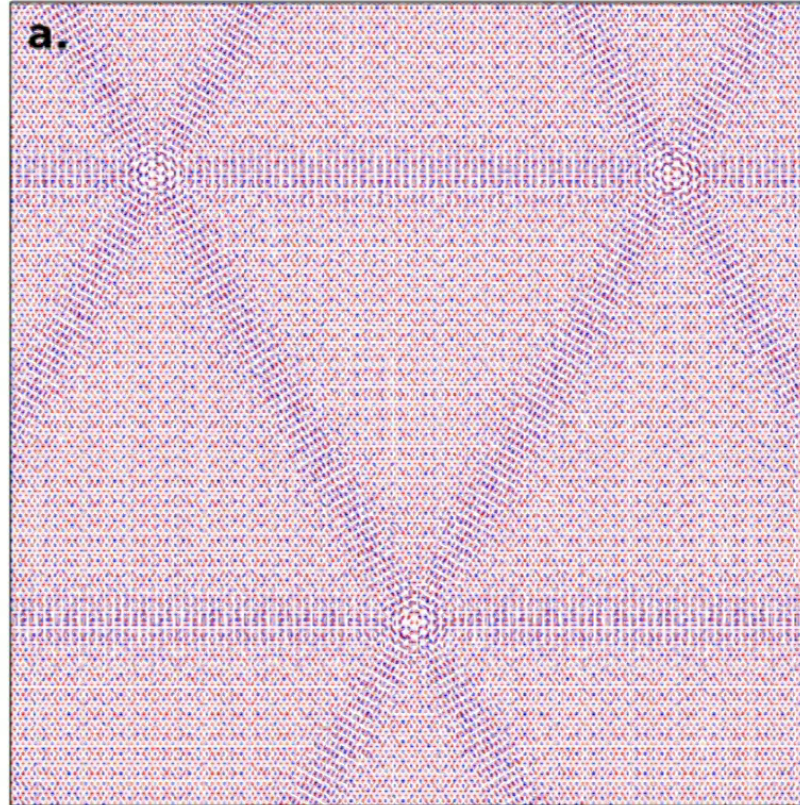


How do atoms of two graphene layers relax ?

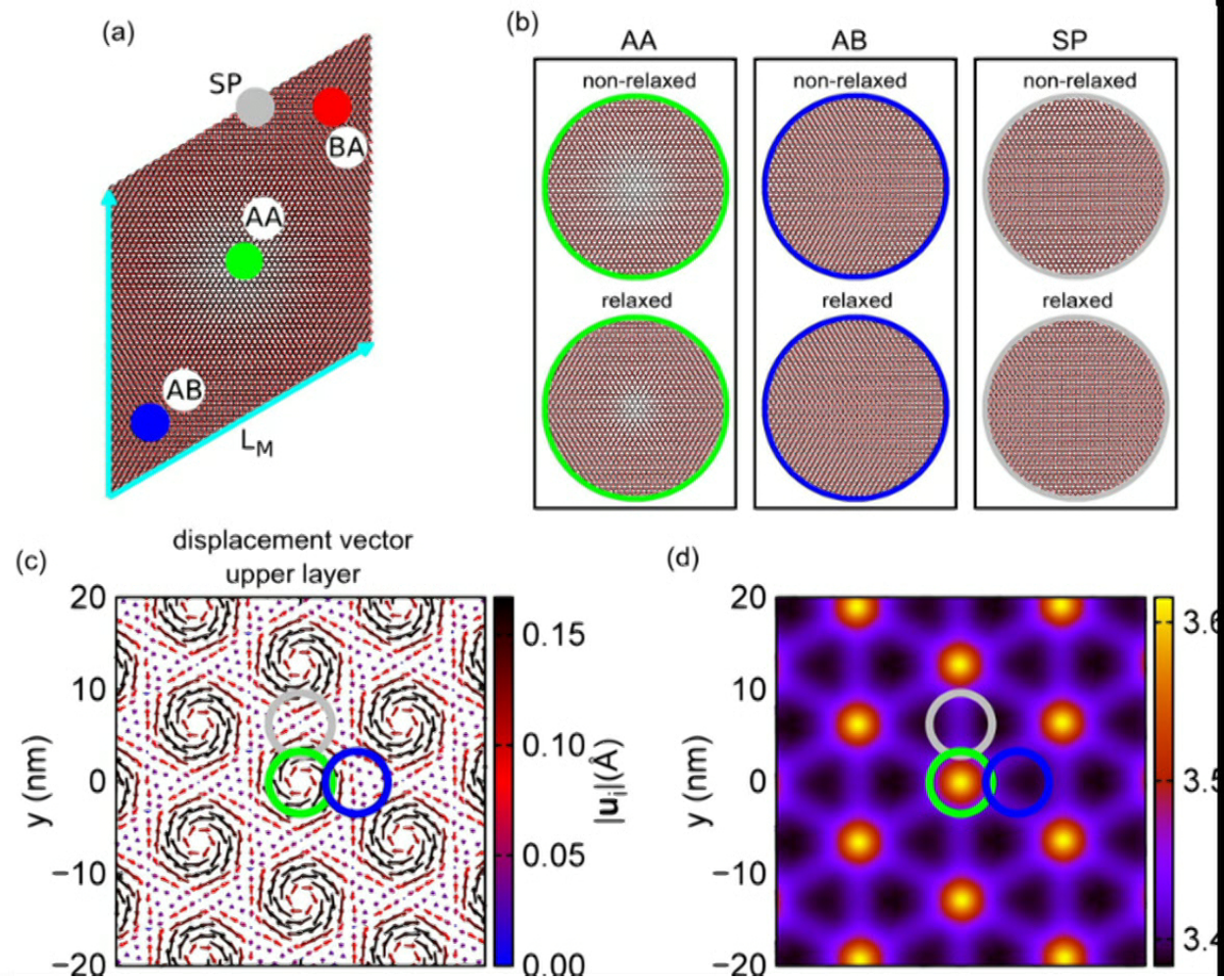


Atomic reconstruction at van der Waals interface in twisted bilayer

Hyobin Yoo et al.
arXiv:1804.03806
(Phil Kim group)



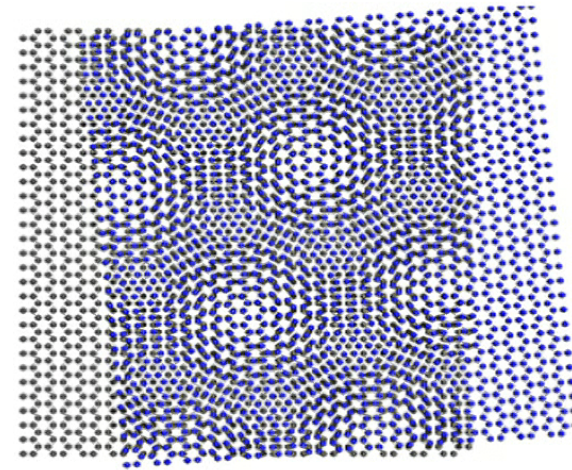
Emergent D 6 symmetry in fully-relaxed magic-angle twisted bilayer graphene
M. Angeli et al., (SISSA group) arXiv:1809.11140



Theory of Emergent Josephson Lattice in Neutral Twisted Bilayer Graphene (Moiré is Different)

arXiv:1804.00627

G. Baskaran



Resonating Valence Bonds in Graphene

How it affects Twisted Bilayer Graphene ?

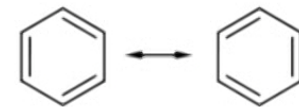
AB stacking as a Mott insulator

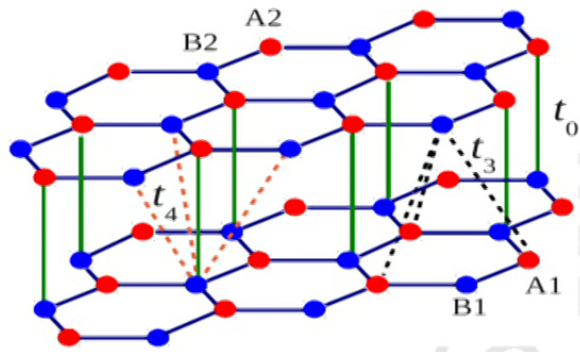
AA stacking, self doping and Cooper pair formation

Triangular lattice Network of Conducting Pathways

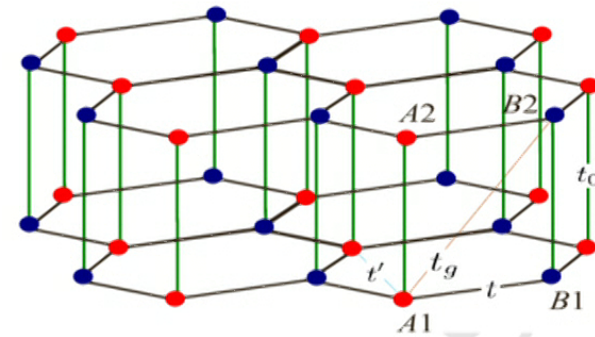
Josephson Tunneling Bose Hubbard Model

Doping via gate voltage produces superconductivity

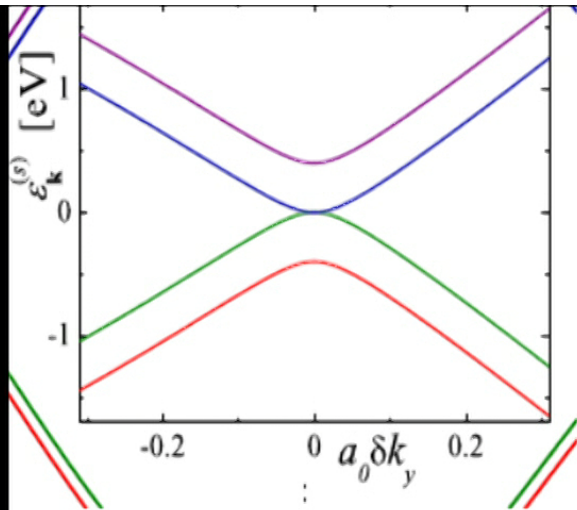




Bernal or AB Stacking



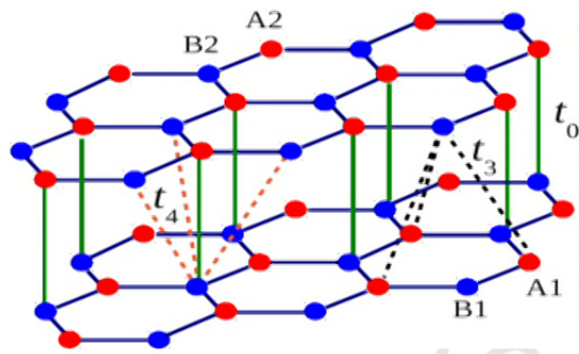
AA Stacking



Consequences of Electron Electron Interactions

In experiments one sees a many body gap of few meV

Theory predicts long range Antiferromagnetic Order (eg. Fu-Chun Zhang et al.)



Bernal or AB Stacking

Consequences of Electron Electron Interactions

No clean experiments available as
AA stacking is unstable

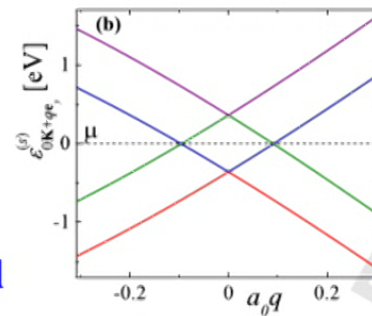
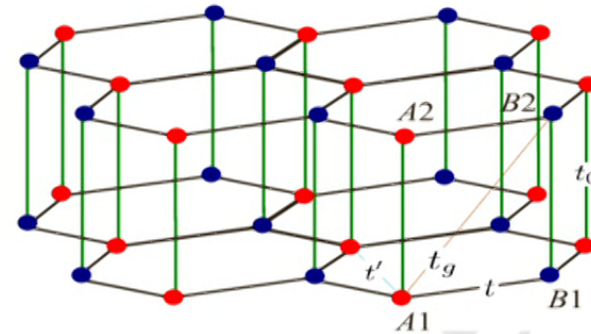
Theory predicts

Exciton liquid (Levitov et al.)

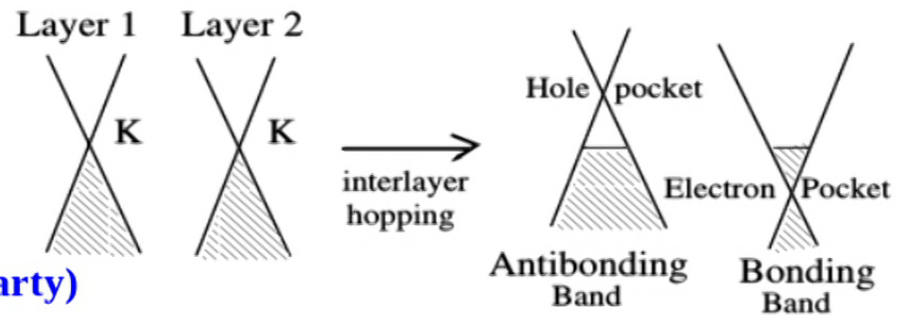
A Cooper pair Exciton ($-2e$, $+2e$) Liquid
(G. Baskaran, to be published)

Pair binding in p-pi bonded
System including C60 molecule

(GB-Tosatti, Kivelson-Chakravarty)



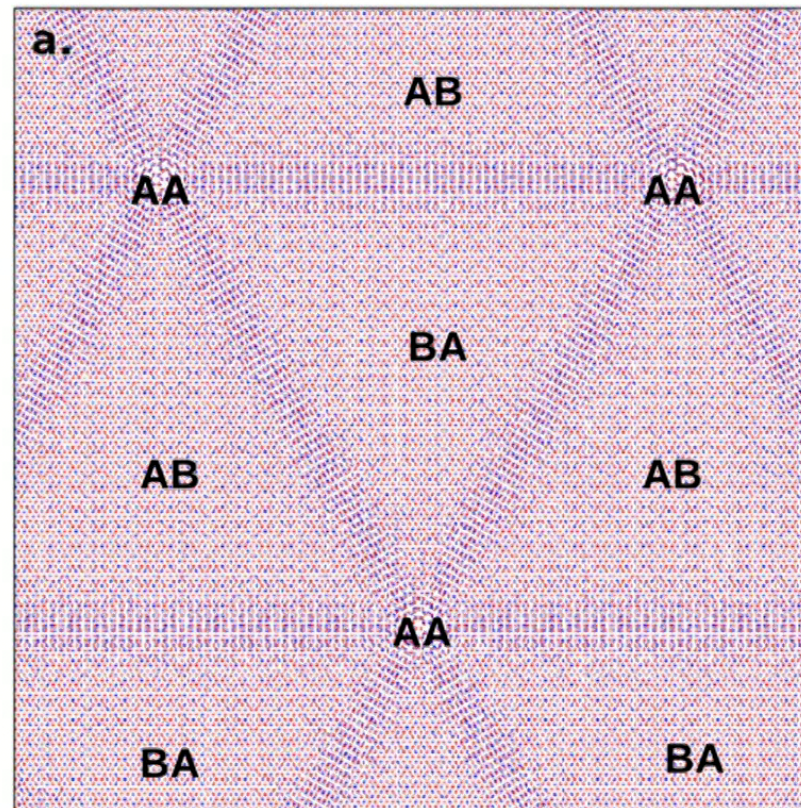
AA Stacking

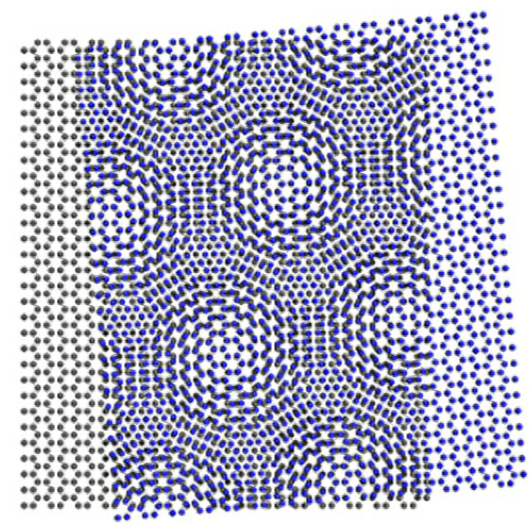
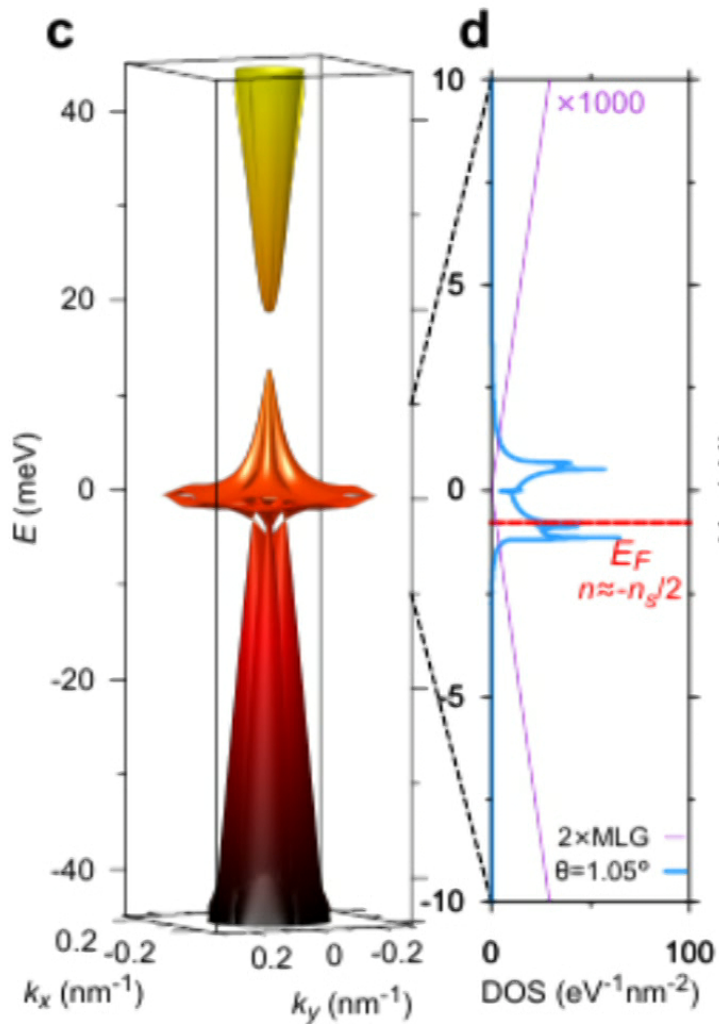


AB and BA
Regions are Mott Insulators

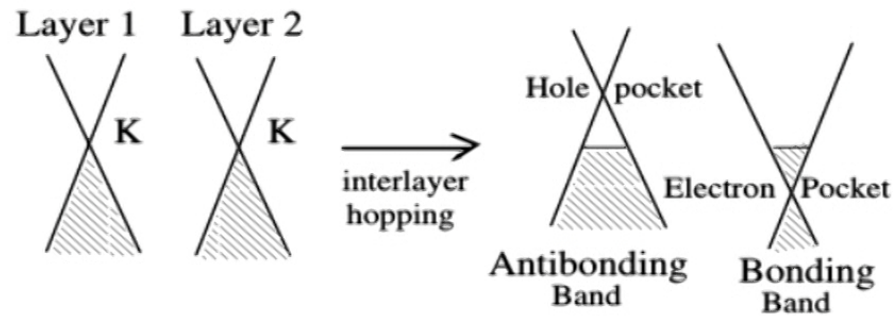
AA region is Metallic

Domain walls are metallic





At the magic angle of 1.16 degree
 number of carbon atoms
 per unit cell is about 2000

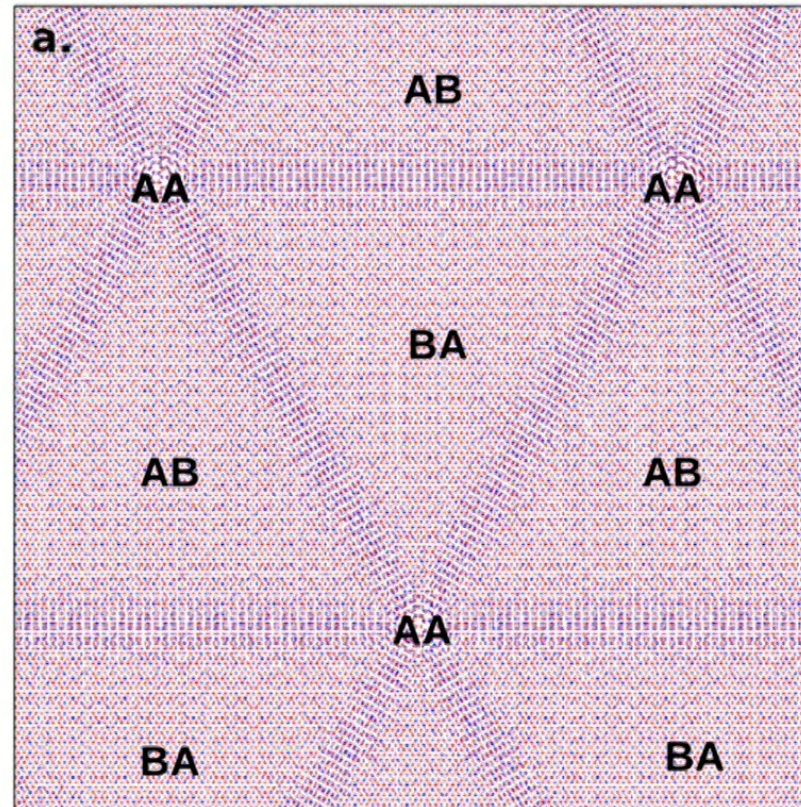


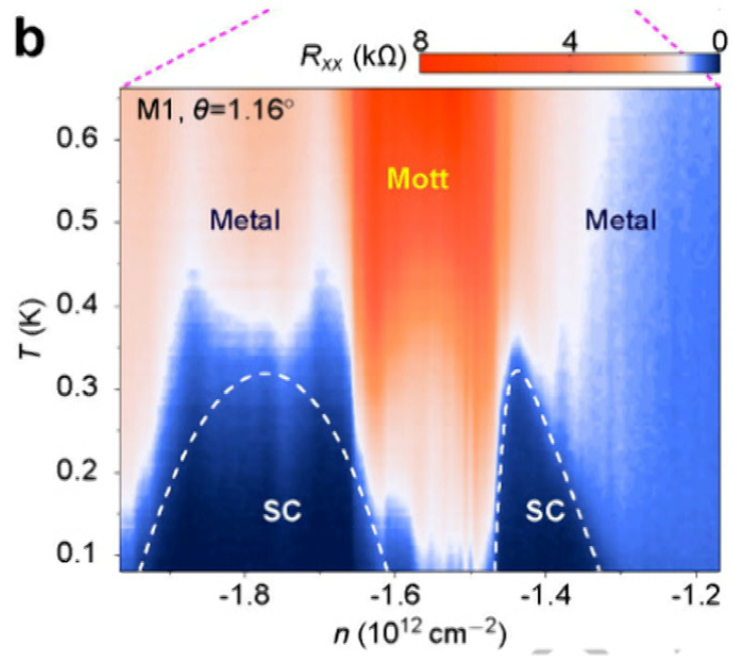
Aerial density of added carriers is $\sim 4 \times 10^{12}/cm^2$. This is very small and is about 0.2 % of density of p_z -electrons $\sim 2 \times 10^{15}$ (or carbon atoms) in neutral graphene layer.

AB and BA
Regions are Mott Insulators

AA region is Metallic

Domain walls are metallic





Conclusions

Our theory predicts

**A Cooper pair Exciton ($-2e$, $+2e$) Liquid
for untwisted AA Bilayer Graphene**

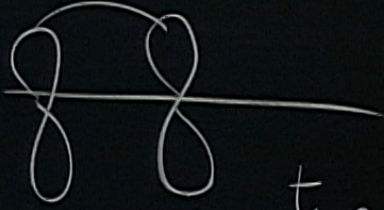
**A predominantly Mott insulating lattice of atoms connected
by conducting walls and vortices**

**Josephson Lattice, a Bose Mott Insulator for TBL graphene
Gate doping induced Bose insulator to Superconductor transtion**

**Exciton Cooper pair liquid to Superconductor transition
induced by bilayer electric field bias in AA graphene and
TBL grapene.**

Presence of shot noise with charge $-2e$ and $+2e$

$t \sim 3\text{eV}$



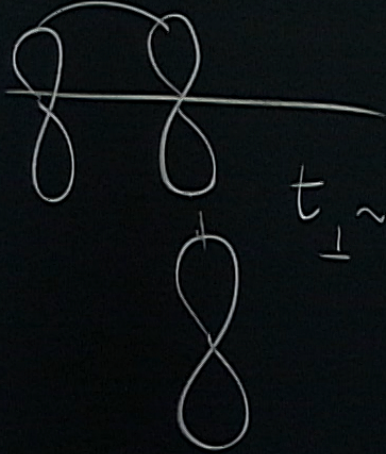
$t_{\perp} \sim 0.3$



Pathak, Sherry & GB

PRB 2012

$t \sim 3\text{eV}$



$t_{\perp} \sim 0.3$

14
10

Pathak, Shenvy & GB

PRB 2012

$2 \times 10^{15} / \text{cm}^2$