Nanometer-Scale Surface and Interface Phenomena

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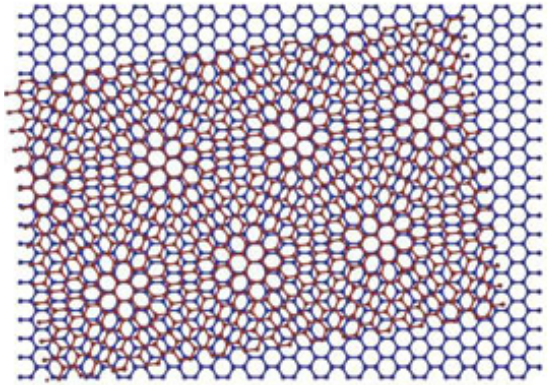
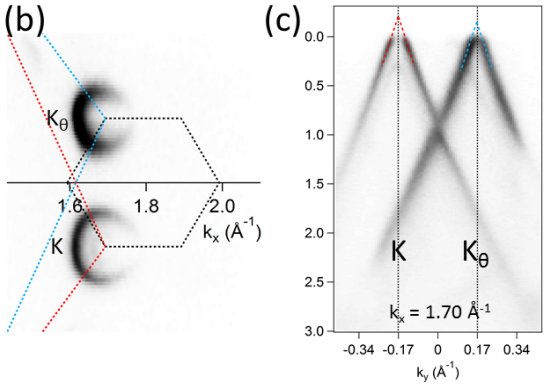
This will be a two-part talk

(1) Programmatic: Brief overview of DOE/BES Program - Nanometer-Scale Surface and Interface Phenomena

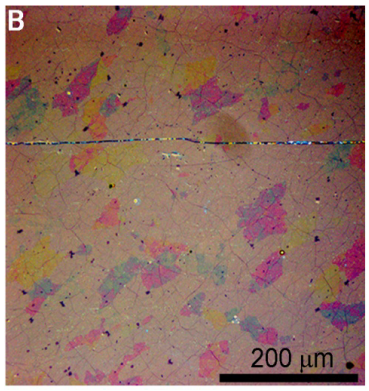
(2) Research Highlight: Structural, electronic, and optical properties of "twisted bi-layer" graphene films



Moiré resulting from stacked layers



Angle resolved photoemission data



Optical micrograph

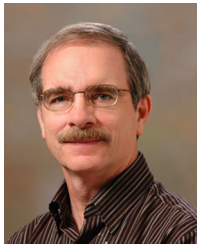
Nanometer-scale surface/interface phenomena team

Research staff


Norm Bartelt


Farid El Gabaly


Peter Feibelman


Gary Kellogg


Kevin McCarty


Nancy Missert

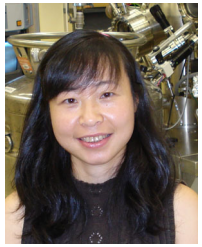

Taisuke Ohta


Brian Swartzentruber


Konrad Thürmer


Kevin Zavadil


Bogdan Diaconescu


Shu Nie

Post-docs


David Siegel


Jey Velmurugan

Task structure and science focus areas

Task structure

1. Atomistic dynamics of surface – Gary Kellogg, PI
2. Collective phenomena in surface dynamics – Norm Bartelt, PI
3. Materials at interfaces: Structural/electronic properties – Peter Feibelman, PI
4. Nanoscale electrochemistry – Nancy Missert, PI

Focus areas

1. Structure and properties of water and ice on solids
2. Growth and properties of 2-D crystals (mostly graphene)
3. Interfacial evolution in energy storage materials
4. Surface dynamics of oxide surfaces and films

Program book: 30 accomplishments and 42 publications (2010-2012)

Research Highlight - Twisted bi-layer graphene (TBG)

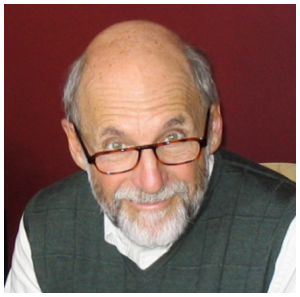
A collaborative effort between Sandia National Laboratories and Naval Research Laboratory

Jeremy T. Robinson (NRL)
Taisuke Ohta, Thomas E. Beechem, Peter J. Feibelman, Bogdan Diaconescu (Sandia)

Taisuke

Jeremy

Thomas



Peter

Bogdan

For details see:

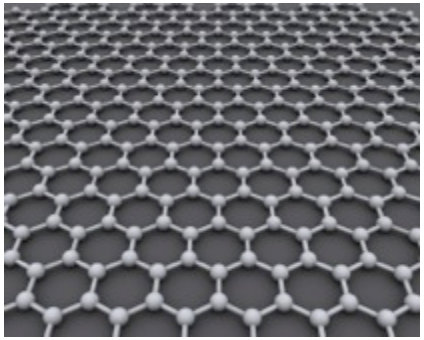
Ohta et al., PRB, 85, 075415 (2012)

Ohta et al., PRL, 109, 186807 (2012)

Robinson et al., ACS Nano, 7, 637 (2013) & Science 152, 374 (2013)

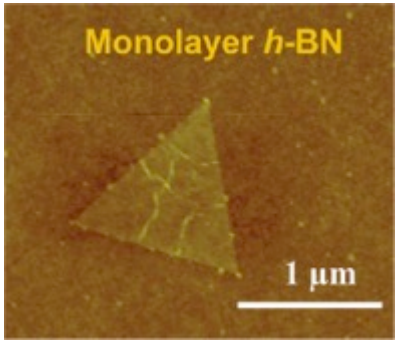
2D crystals – A new class of materials

Number of 2D materials is increasing



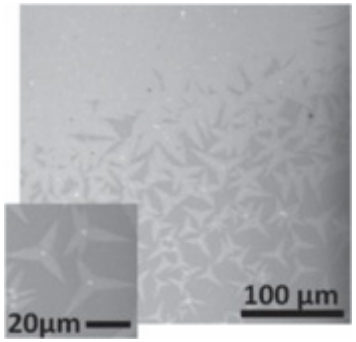
Graphene

http://en.wikipedia.org/wiki/Graphene



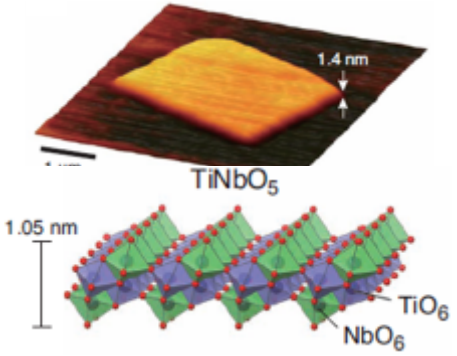
Boron nitride

Kim et al., Nano Lett., 12, 161 (2012)



Molybdenum disulfide

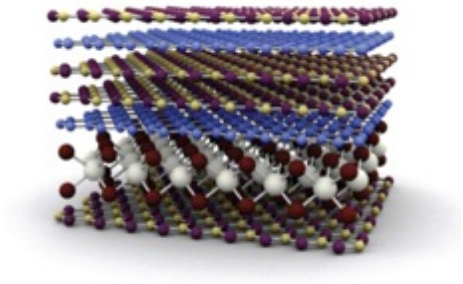
Lee et al., Advanced Materials, 24, 2320 (2012)



Titanium Niobate

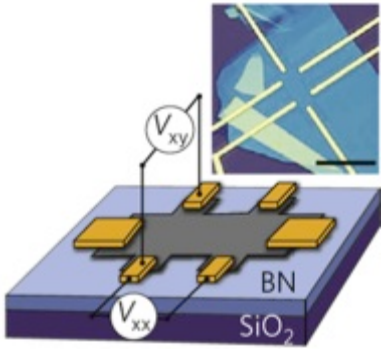
Osada et al., Adv. Funct. Mater. 21, 3482 (2011)

Hybrid 2D materials offer even greater potential for new properties



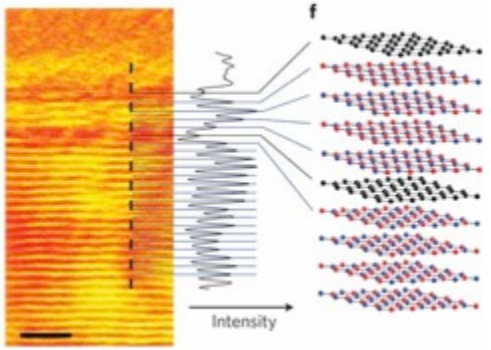
2D-based heterostructure

Novoselov et al., Nature 490, 192 (2012)



Graphene on BN

Dean et al., Nature Physics 7, 693 (2011)

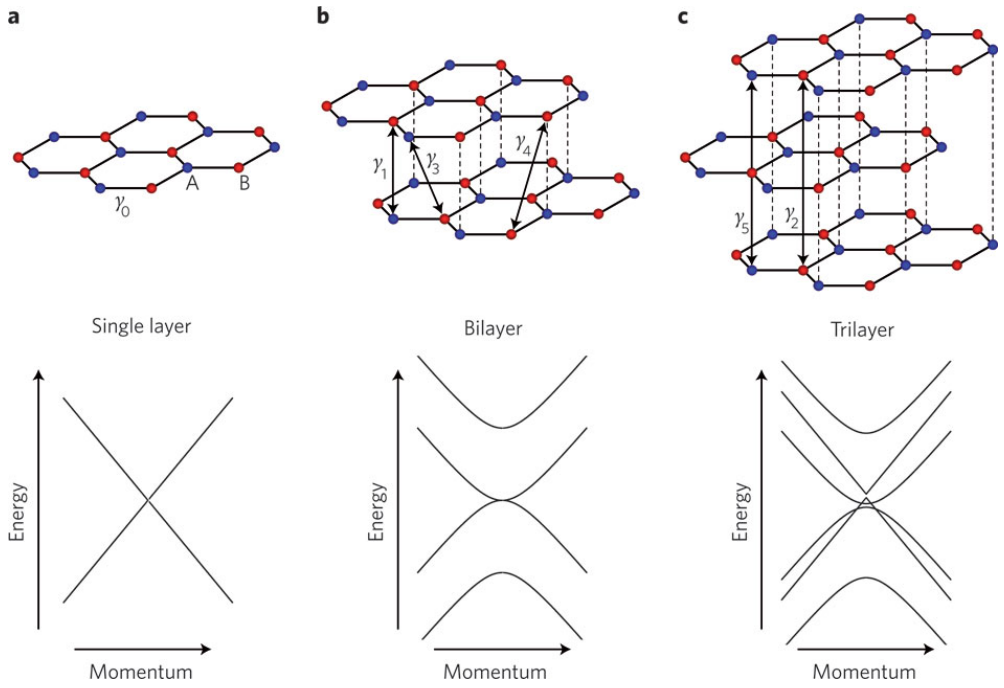


Graphene/BN superlattice

Haigh et al., Nature Materials 11, 764 (2012)

Electronic dispersion of graphite is sensitive to coupling

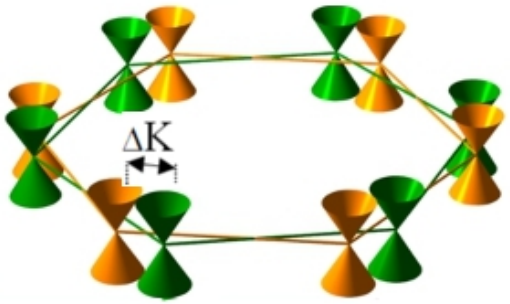
Bernal stacked graphene: layers interact



Freitag, Nature Physics 7 596 (2011)

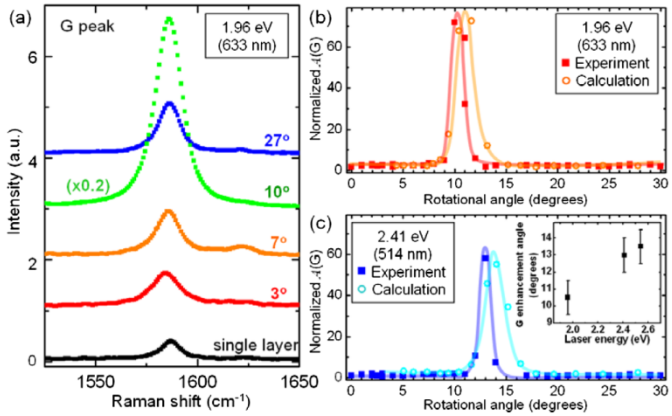
How does azimuthal misorientation change interactions?

Simplified picture of overall Brillouin zone – no interactions



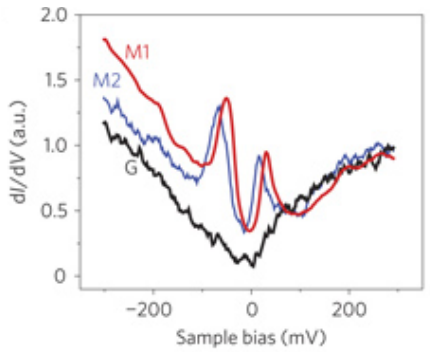
http://www.physics.rutgers.edu/~aluican/research.html

Raman shows resonant transition due to vHs or parallel states

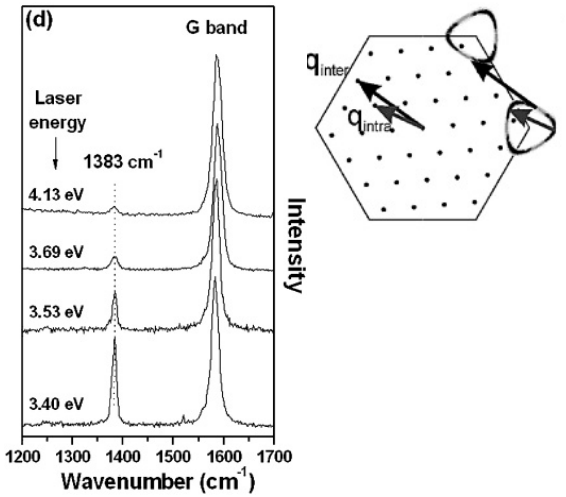


Kim et al., PRL 108, 246103 (2012)

STS indicates van Hove singularities (vHs)



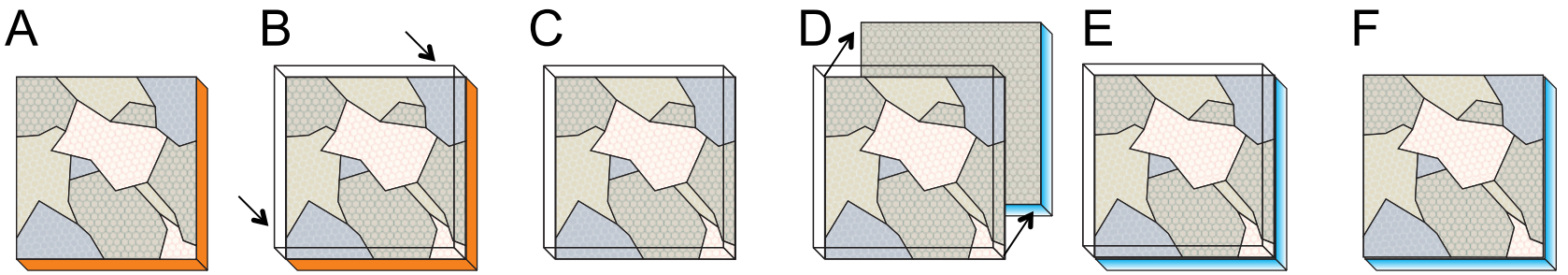
Li et al., Nature Physics 6, 109 (2010)



Righi et al., PRB 84, 241409(R) (2011)

The making of twisted bilayer graphene (TBG)

Transferring CVD graphene onto epi-graphene (on SiC) yields large TBG domains with various twist angles



–Monolithic epi-graphene
–Large-domain CVD graphene (>100um-size domain)

CVD graphene

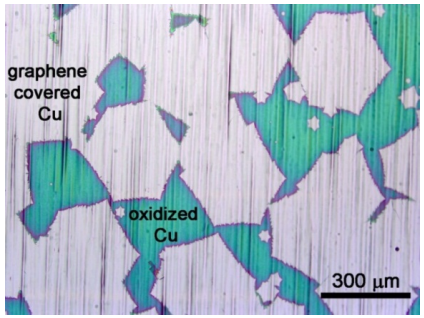
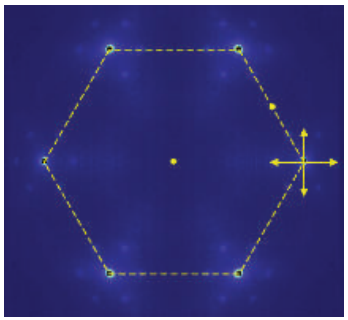
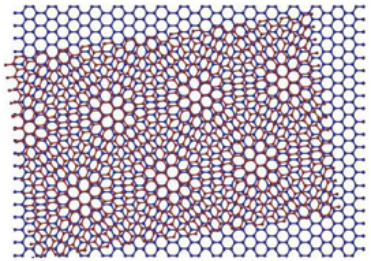


Figure courtesy: Jeremy Robinson

Epi-graphene on SiC(0001)

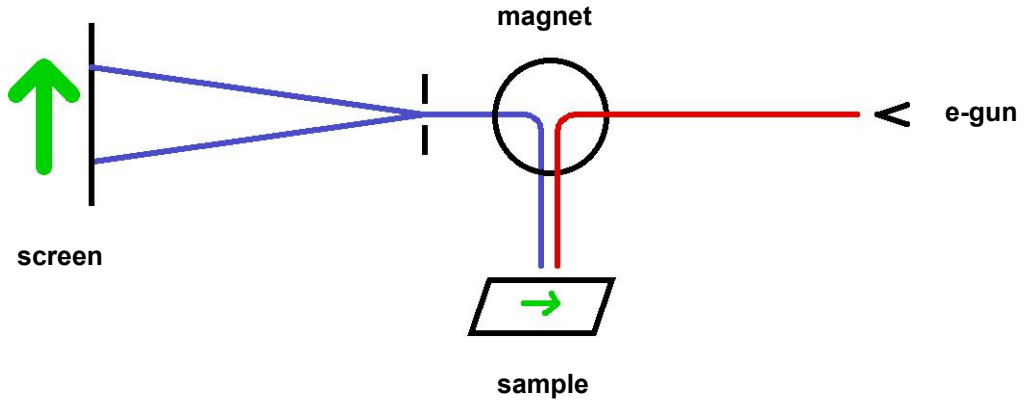


Bostwick et al., Nature Phys. 3, 36 (2007)

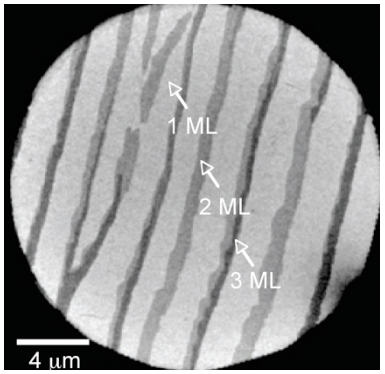


Really?

Low energy electron microscopy (LEEM)

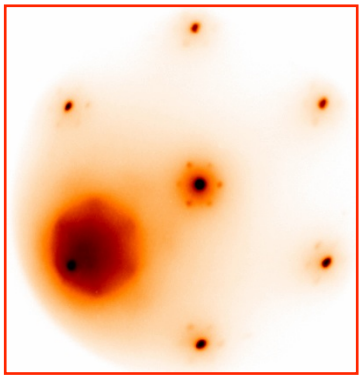


Surface morphology



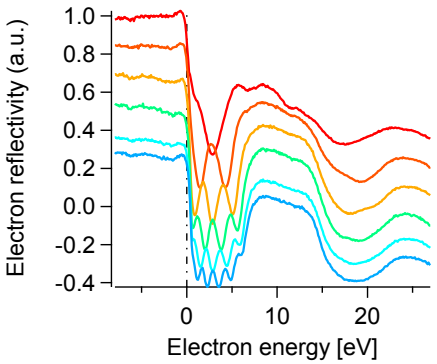
LEEM

Atomic structure



LEED

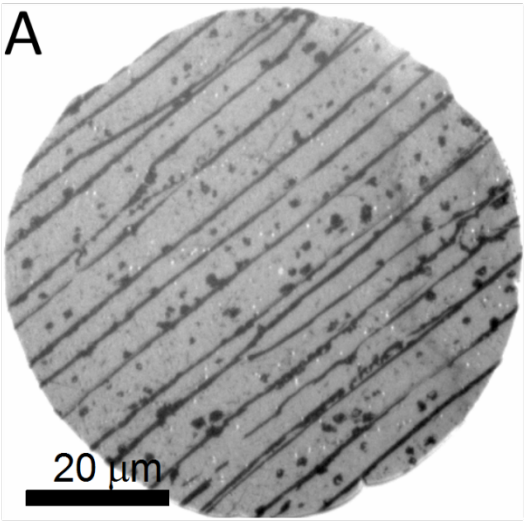
Layer thickness



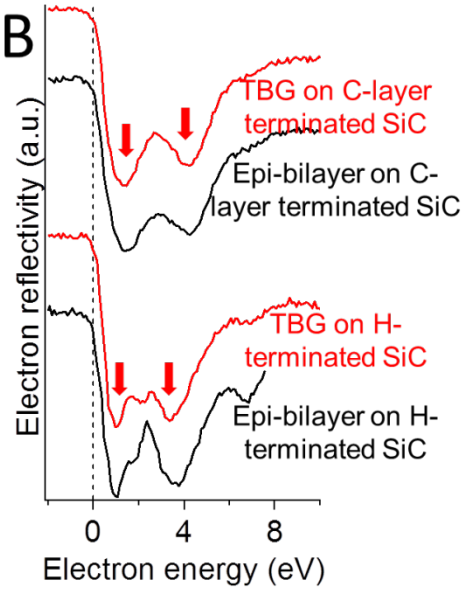
LEEM-IV

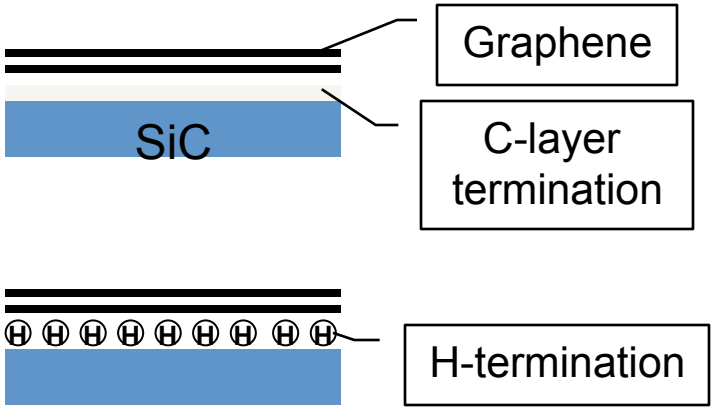
Reflectivity curves are characteristic of bilayer graphene

- Two dips in electron reflectivity spectra: bilayer graphene on SiC
  - Low energy electron microscopy (LEEM) measurement



LEEM image of TBG



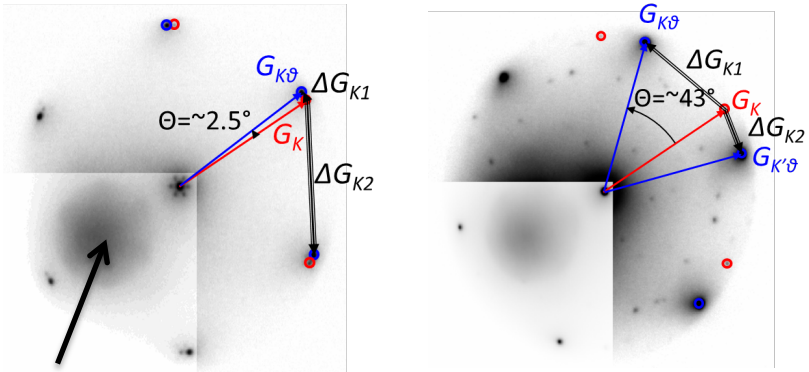


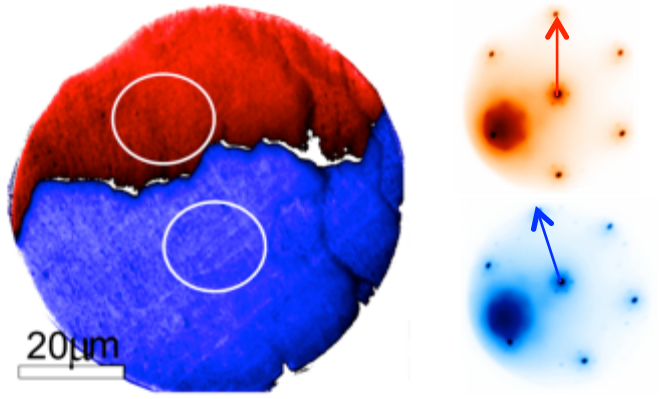
Ohta et al., PRB, 85, 075415 (2012)

Minimum damage of graphene was confirmed using Raman spectroscopy

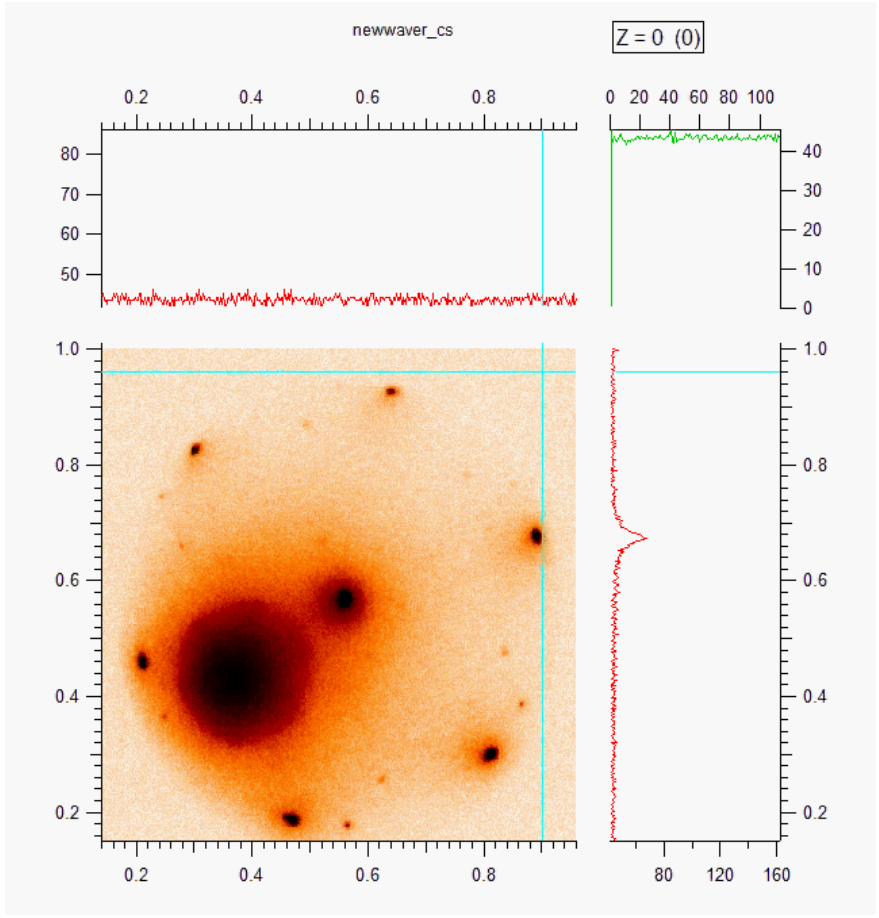
LEED confirms azimuthal misorientation

- Underlayer diffraction spots
- Overlayer diffraction spots





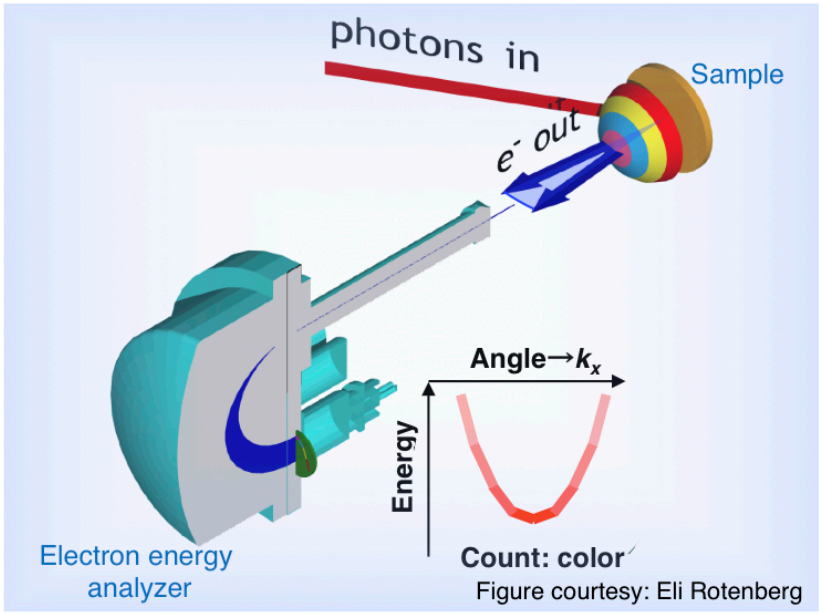
Domain size is 10s of microns



Movie: Translate sample under electron beam

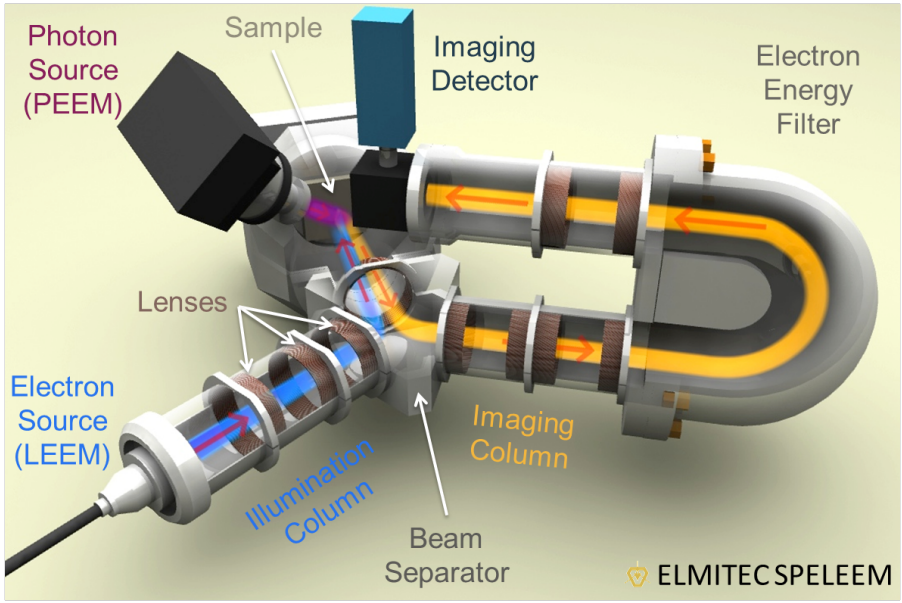
How do we characterize electronic structure?

Angle-resolved photoemission spectroscopy (ARPES) measures dispersion of occupied electronic states

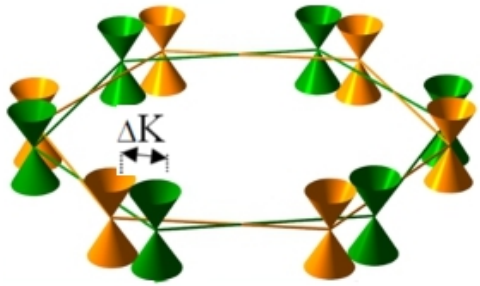


← "Conventional" ARPES

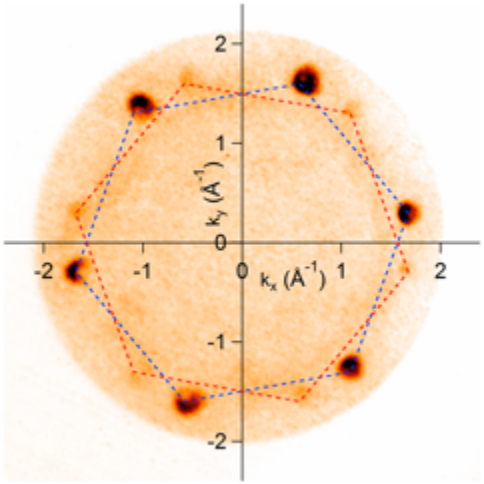
Spectroscopic LEEM-PEEM
(New capability funded by BES) →



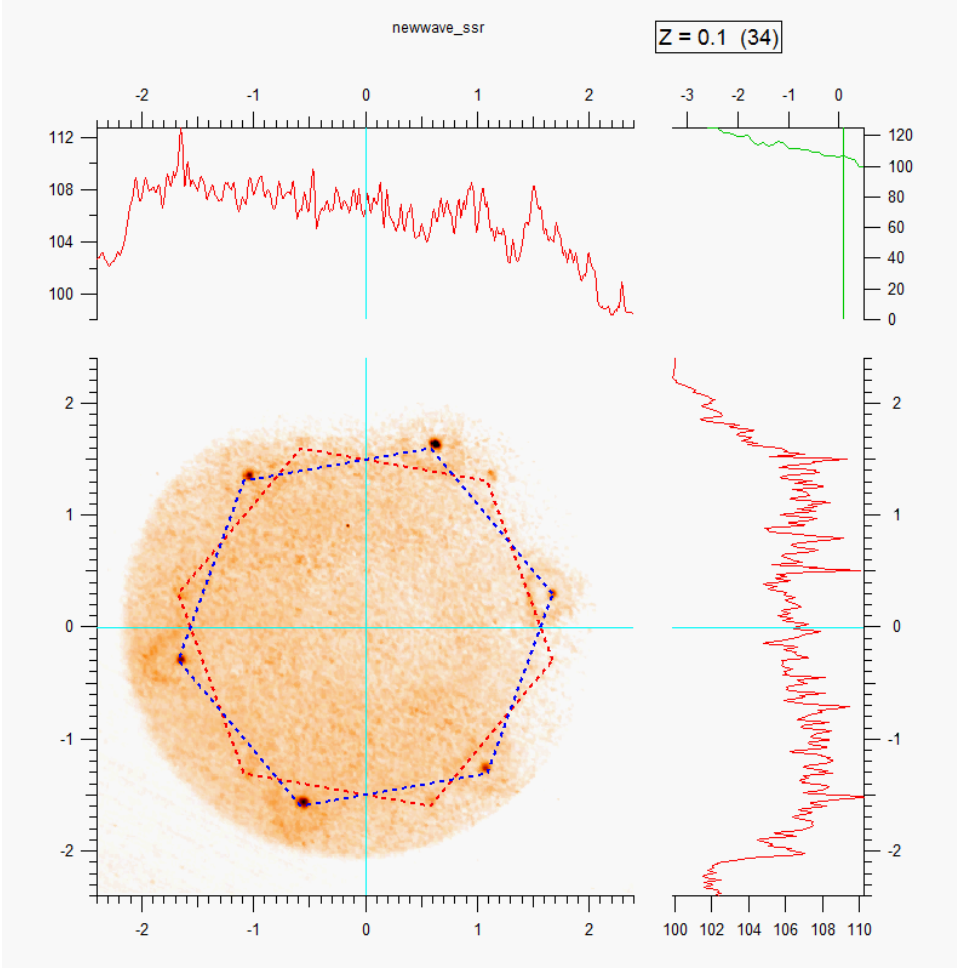
PEEM consistent with simple picture



http://www.physics.rutgers.edu/~aluican/research.html

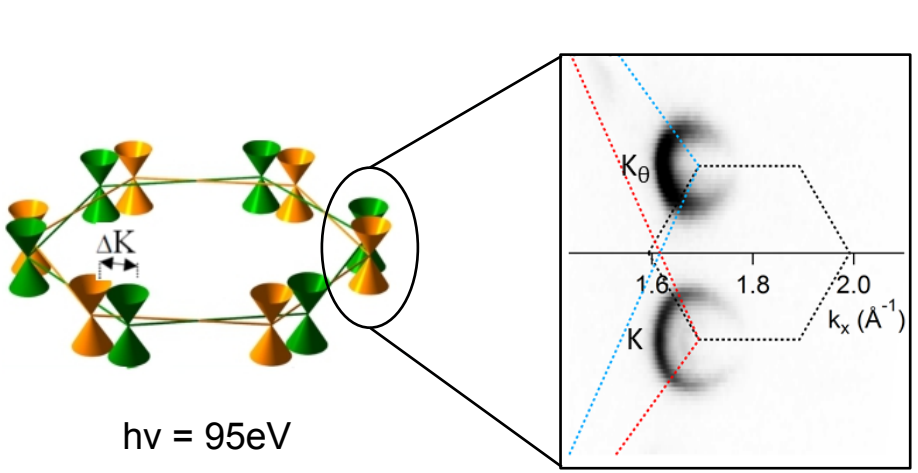


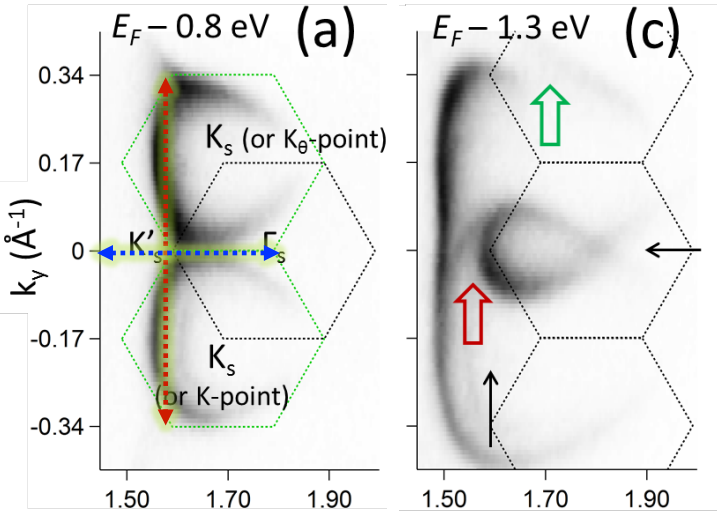
Angular distribution measured in Spe-LEEM-PEEM (hν=20 eV)

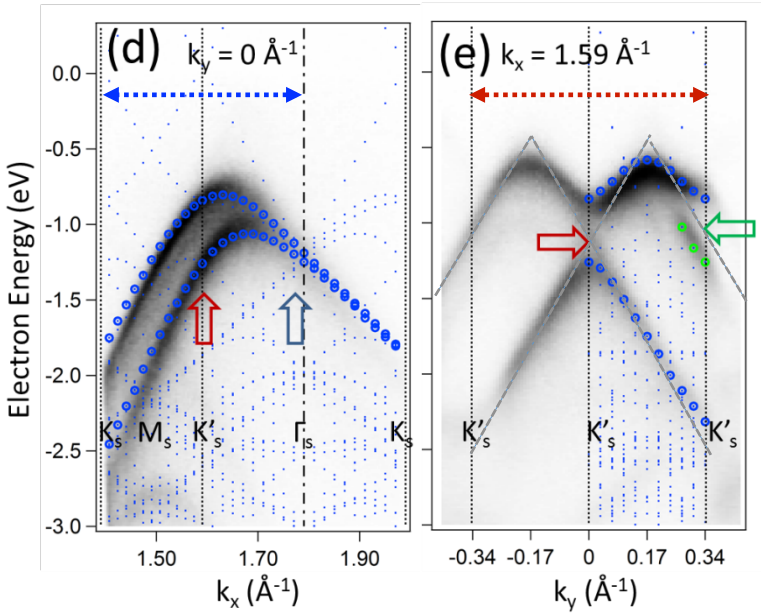


Movie: Stacked energy slices (Dirac cones)

Synchrotron ARPES: Twisted bilayers interact

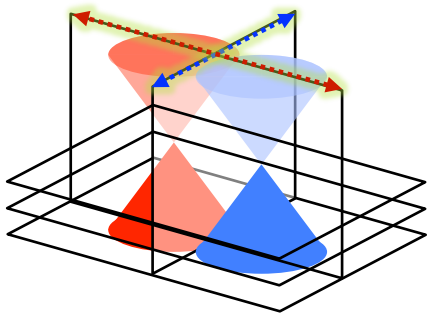






Blue dots/circles: DFT calculation

Additional feature
at the green arrow



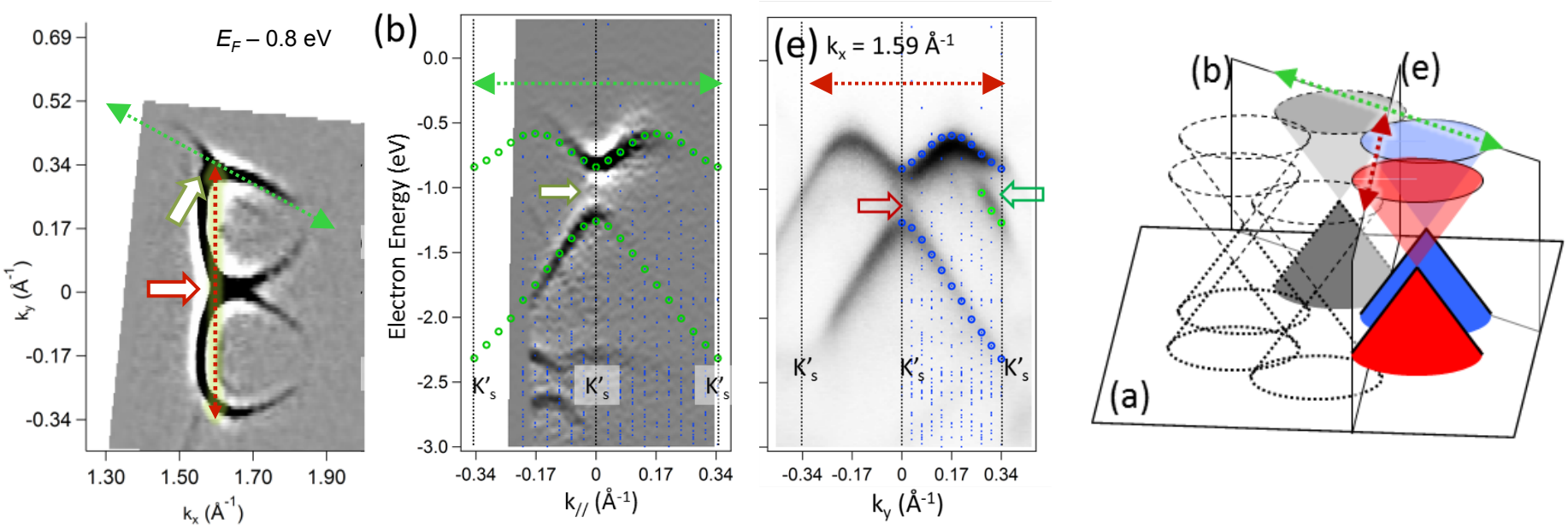
Two cones' interaction leads to mini-gap and van Hove singularities

Match well with DFT calculation

Ohta et al., PRL, 109, 186807 (2012)

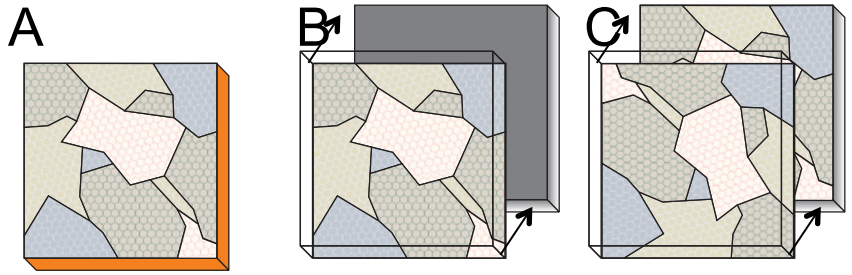
Additional Dirac cones emerge

Anti-crossing is found between the original and the additional Dirac cones

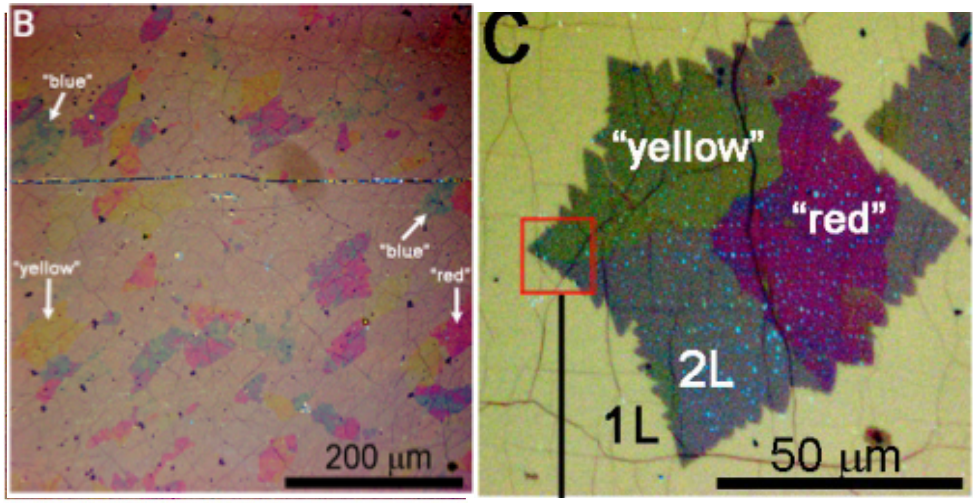


Does band renormalization affect TBG properties?

Double transfer of CVD graphene on to SiO_2/Si substrate



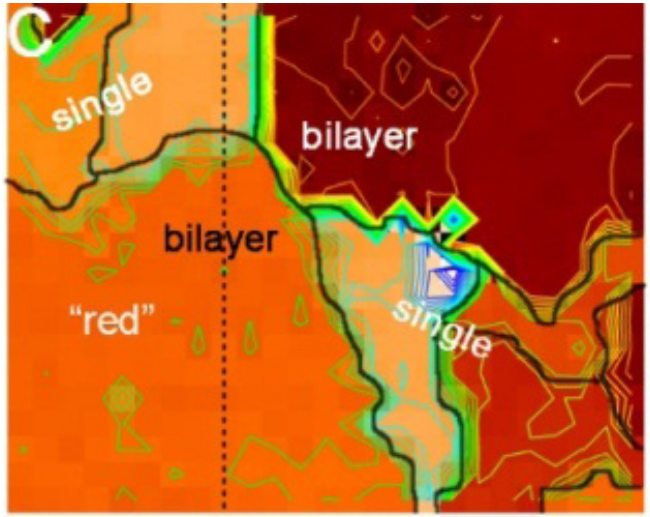
Colored patches observed in optical microscope for TBG on SiO_2/Si substrate



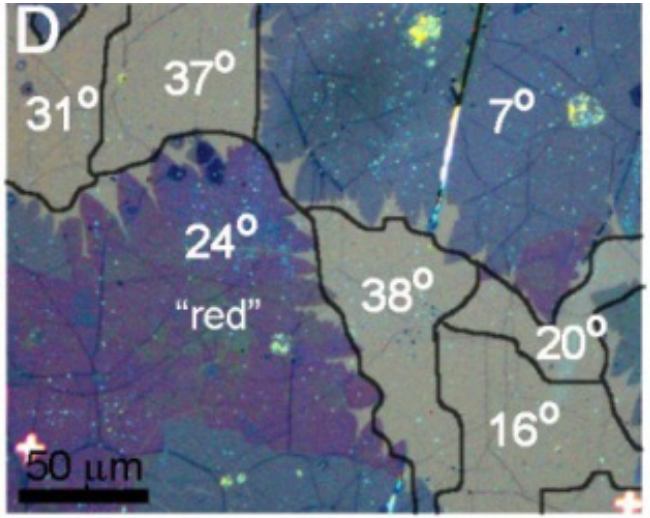
Robinson et al., ACS Nano, 7, 637 (2013) & Science 152, 374 (2013)

Optical absorption depends on the twist angle

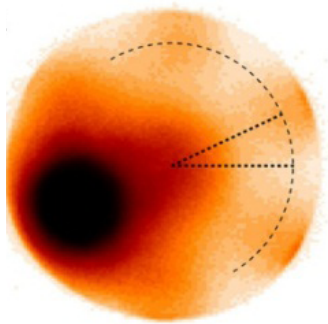
Low energy electron diffraction (LEED) shows direct correlation between the color and the twist angle



Map of LEED pattern orientations across the sample surface

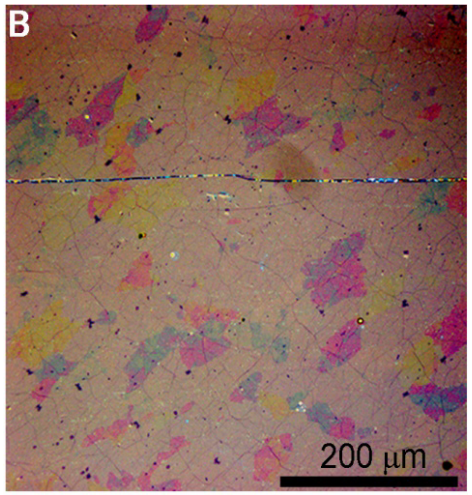


Optical micrograph of the same area

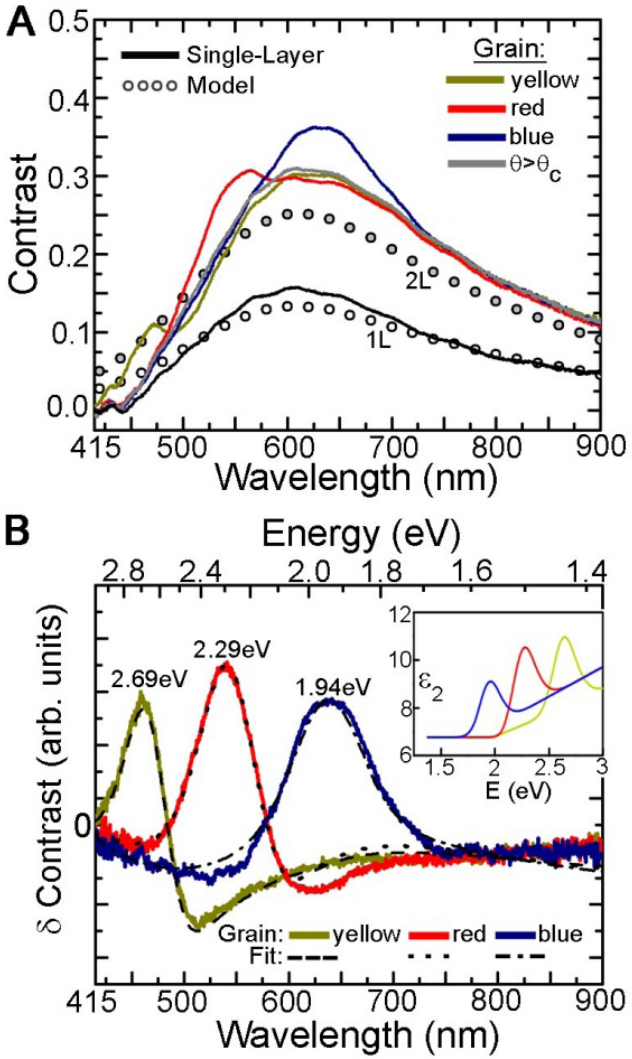


Typical µ-LEED pattern of TBG

Emerging absorption band responsible for colored areas



Optical spectroscopy reveals an absorption band for colored regions



Summary

- Twisted Bilayer Graphene (TBG) can be produced using transfer method
- Domains have varying twist angles
- Domain size large enough to probe properties (tens of microns)
- Angle-resolved photoemission show interlayer electronic interactions
- Electronic dispersion is altered by moiré (long-range periodicity)
- Moiré is ubiquitous feature in 2D-solids: handle to tailor electronic properties
- Optical properties can be tuned by the twist angle

Acknowledgements

- Collaborators (in addition to those whose photographs appeared earlier):
  - R. G. Copeland, A. McDonald, N. C. Bartelt, K. McCarty, S. Nie, E. Loginova (Sandia National Laboratories)
  - S. Schmucker, J. C. Culbertson, J. P. Long, A. Friedman (Naval Research Laboratory)
  - A. Bostwick, E. Rotenberg (Lawrence Berkeley Laboratory)
- User facility:
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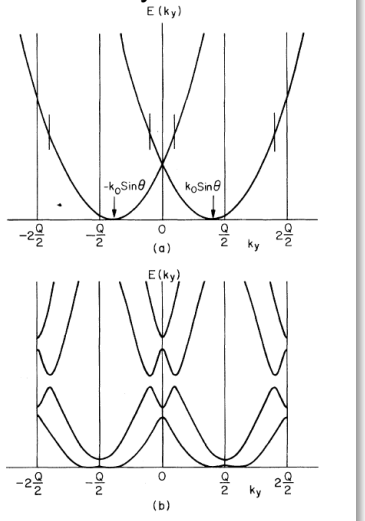
Superlattice changes electronic dispersion

Substrate or neighboring material provides periodic potentials

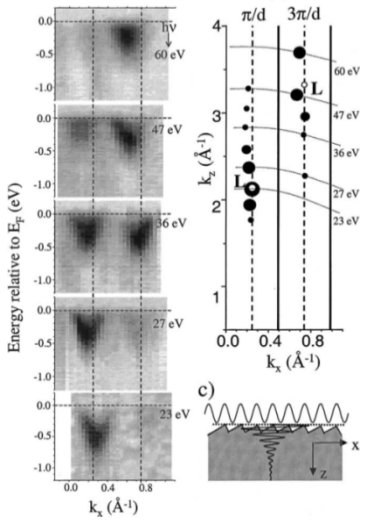
Surface superlattice

Mini-bands & gaps formed in inversion layer of vicinal Si



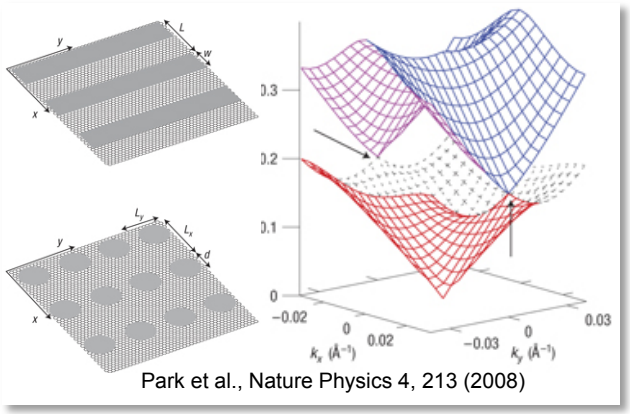
Tsui et al., PRL 40, 1667 (1978)

Surface state on Au(322) vicinal surface



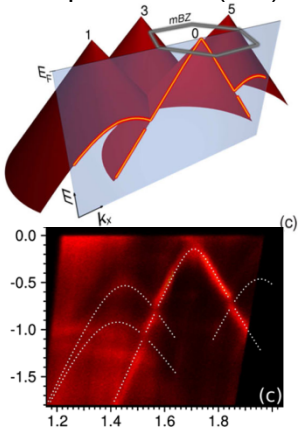
Ortega et al., Materials Science and Engineering B96 154 (2002)

Graphene superlattice



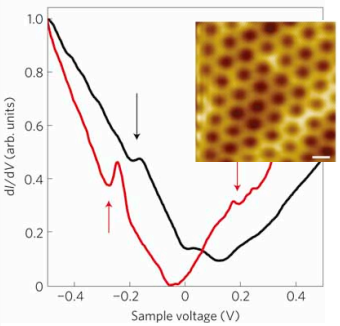
Park et al., Nature Physics 4, 213 (2008)

Graphene on Ir(111)



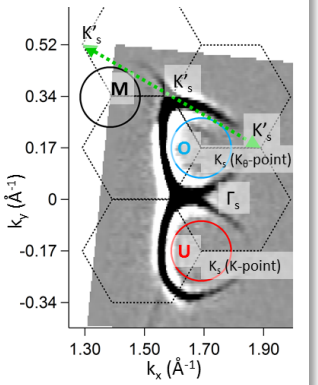
Pletikosic et al., PRL 102, 056808 (2009)

Graphene on hBN



Yankowitz et al., Nature Physics 8, 382 (2012)

Twisted bilayer graphene



Moiré is ubiquitous in hybrid 2D-crystal stacks