GRAPHENE AND 2DM VIRTUAL CONFERENCE & EXPO

10 ANNIVERSARY

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Strain and correlations on flat bands of TBLG in STM Measurements

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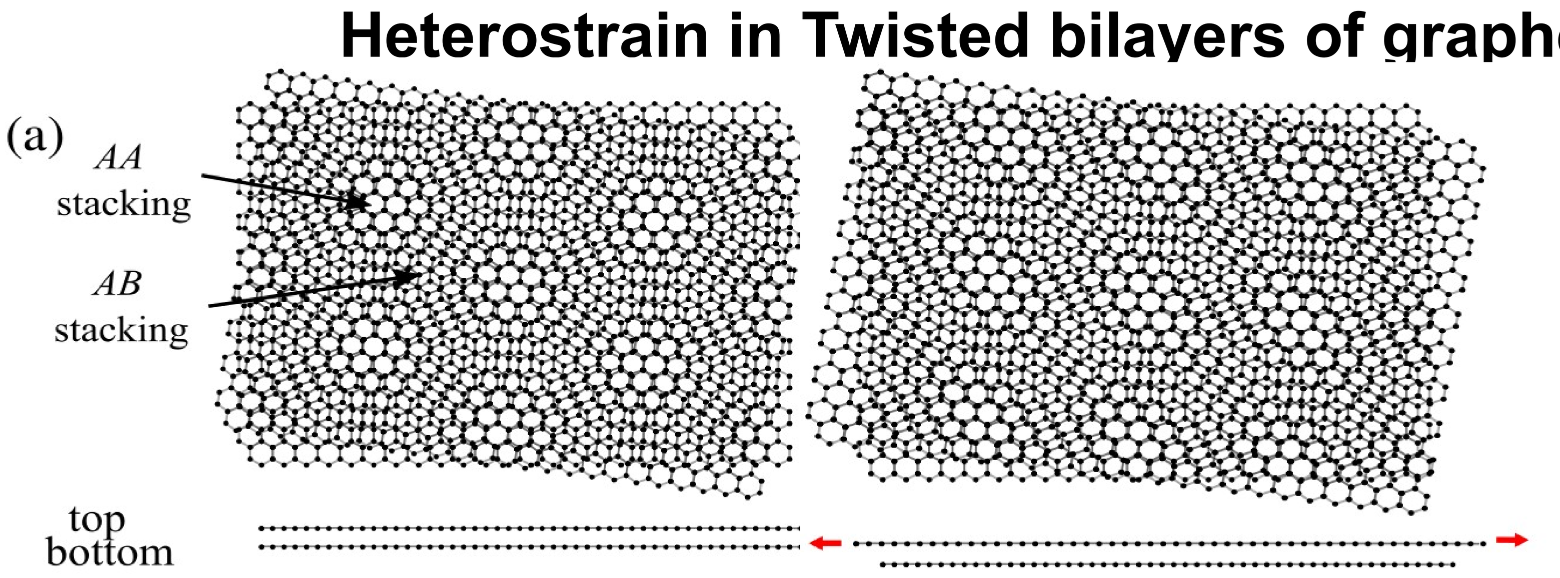
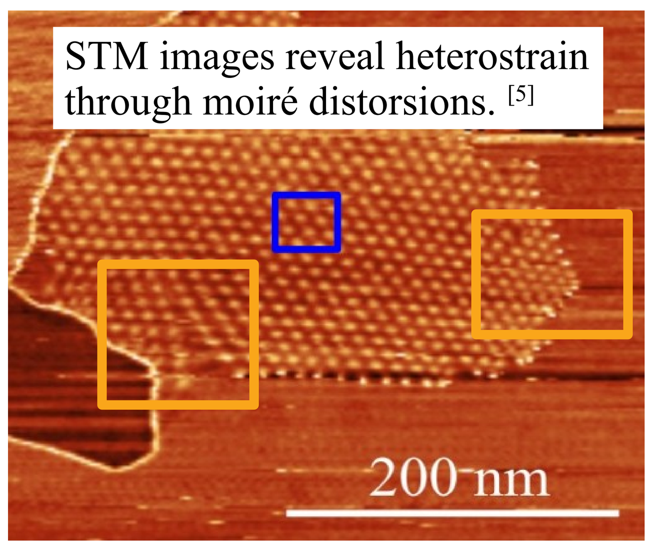
Introduction

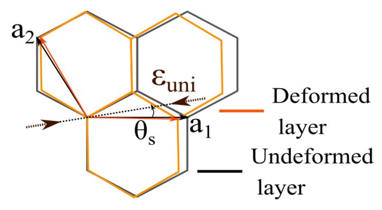
In twisted bilayers of graphene (TBLG), the two layer's graphene periodicity interfere in a moiré pattern that is characteristic of their precise stacking arrangement [1, 2]. For low angles (~1.1°), the charge carriers posses no kinetic energy, thus enhancing correlations between the electrons and yielding the formation of novel correlated states [3,4]. Here we survey recently published STM (Scanning Tunneling Microscopy) measurements Ref. [5-13] showing that for such low angles the physics are controlled first by heterostrain *i.e.* the relative strain between the two layers, small angle variations acting on top of that. We show that even small details in heterostrain can have dramatic effect on the flat bands, and enable to describe all available STM experiments for highly doped samples. When the energy of electrons lie in the flat bands however, the system enters a new regime that is not captured by Hartree Fock calculations, though they include strain and electronic interactions.

Heterostrain in Twisted bilayers of graphene (TBGL)



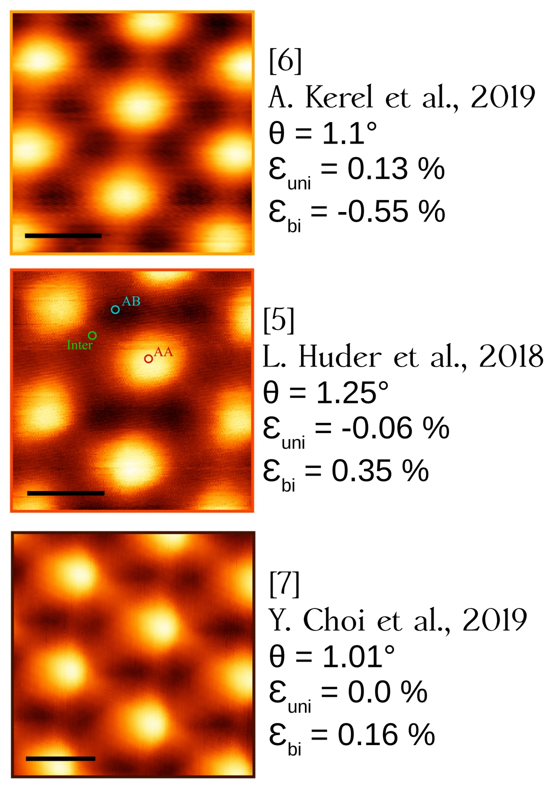


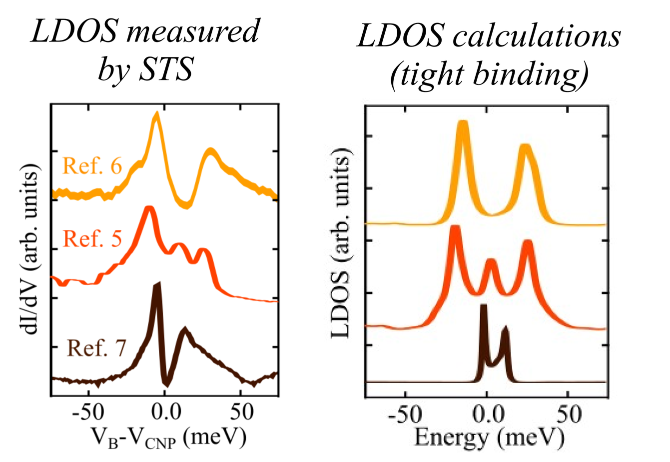
Heterostrain is the relative stacking of the layers : top layer (a_{t1}, a_{t2}) is described as a transformation of the botom layer (a_{b1}, a_{b2}) including rotation $\theta \sim \theta_1 - \theta_2$, uniaxial strain ε_{uni} in a given direction $\theta_s = -\theta_1$, and biaxial strain ε_{bi}. [5, 14]



$$\begin{pmatrix}a_{t_1}\\ a_{t_2}\end{pmatrix} = \begin{pmatrix}\cos\theta_2 & -\sin\theta_2\\ \sin\theta_2 & \cos\theta_2\end{pmatrix}\begin{pmatrix}(\varepsilon_{uni}+1) & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\cos\theta_1 & -\sin\theta_1\\ \sin\theta_1 & \cos\theta_1\end{pmatrix}\begin{pmatrix}(\varepsilon_{bi}+1) & 0\\ 0 & (\varepsilon_{bi}+1)\end{pmatrix}\begin{pmatrix}a_{b_1}\\ a_{b_2}\end{pmatrix}$$

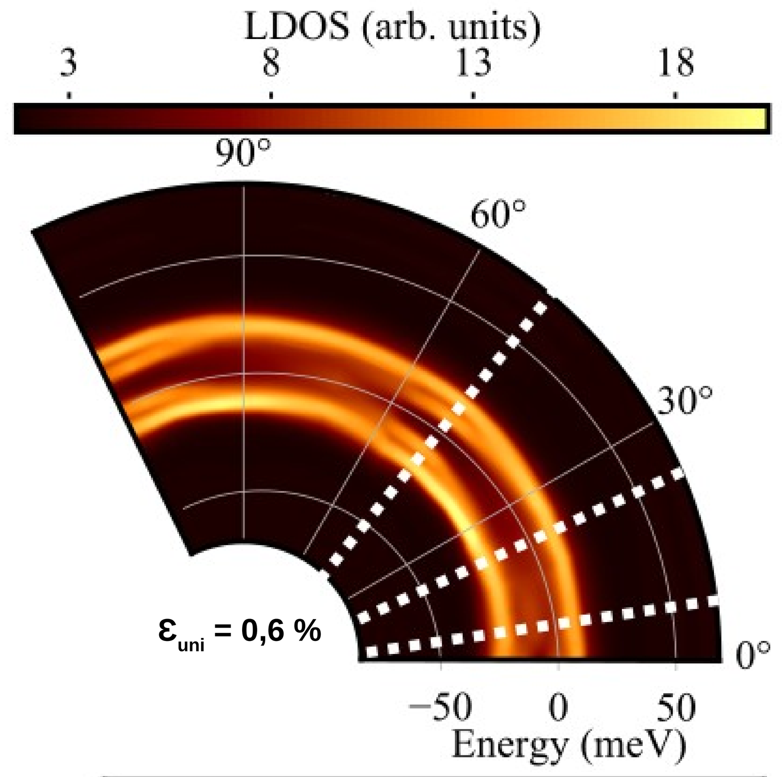
STM topographic images revealing quite similar structures, yet with very different electronic properties as shown by spectroscopy measurements.





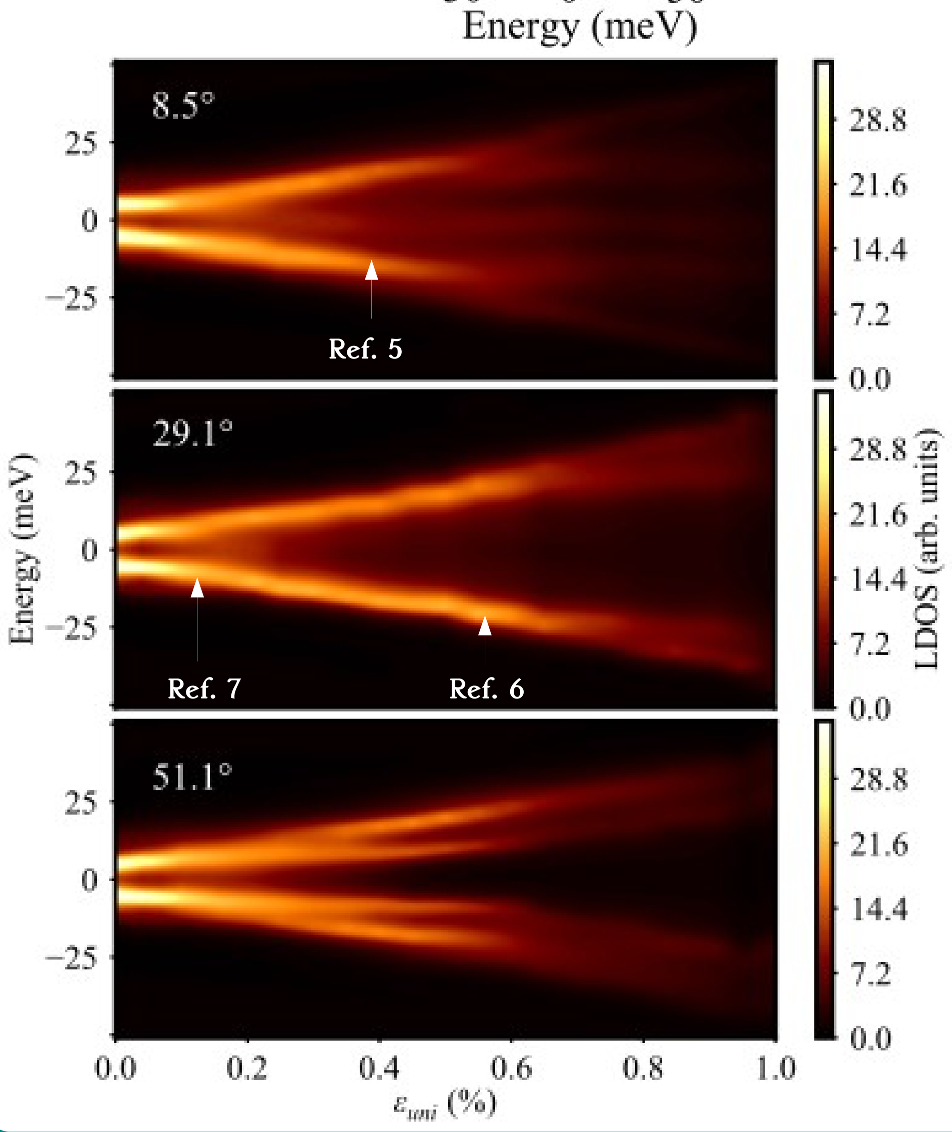
The physics are well understood when including the exact stacking between the layers.

Strain effect for TBLG rotated by 1.1°



When the angle of application of uniaxial strains varies, 3 different behaviours of the LDOS can be distinguished :

- θ_s ~ 8.5° : a zero energy peak of high density of states appears ;
- θ_s ~ 30° : two simple vHs appear ;
- θ_s ~ 51° : the two vHs are splitted appart.

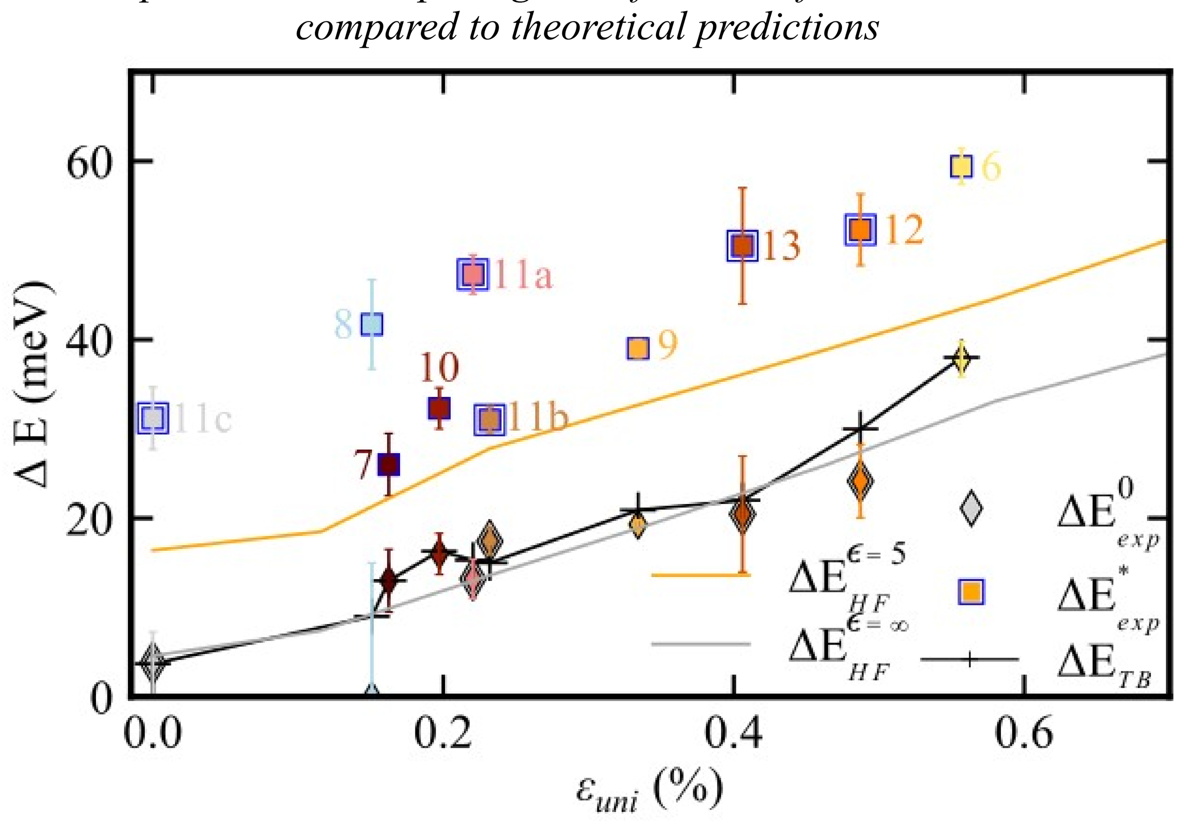


Heterostrain alters the flat bands of low angle TBLG because it occurs in a Van der Waals stacking that has no interlayer chemical bonds (unlike for cuprates for ex), creating a relative displacement of the atomic lattice that accumulates over large superlattices (> 100 nm²), and making its effect non negligible even for small values.

vHs spacing increases linearly when uniaxial strain is increased ~50meV/%

Meta-analysis of recent STM experiments

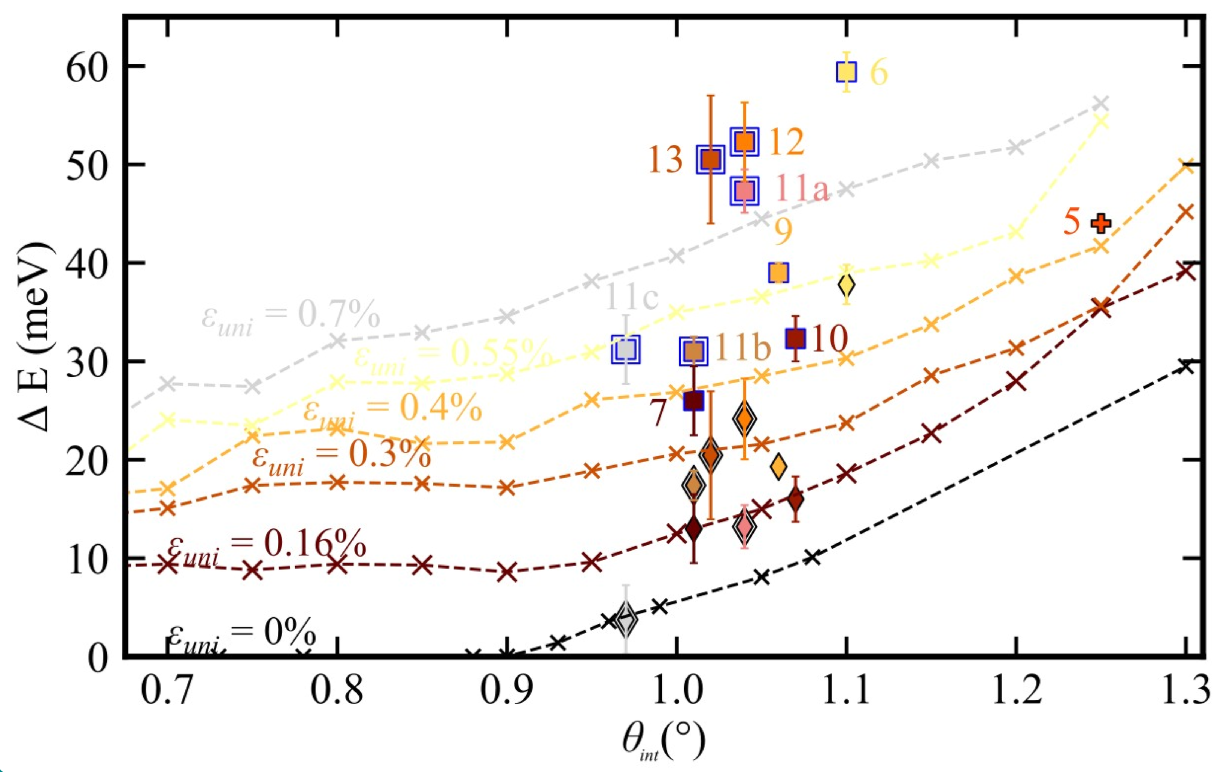
Experimental vHs spacings as a function of uniaxial strain, compared to theoretical predictions



For high dopings, experiments (ΔE^0_{exp}) show a linear trend well described by tight binding (ΔE_{TB}) and Hartree Fock calculations ($\Delta E^{\varepsilon=\infty}_{HF}$) that include strain.

Close to CNP, Hartree Fock calculations ($\Delta E^{\varepsilon=5}_{HF}$) including strain and coulomb interactions underestimate the vHs spacing. Experiments (ΔE^*_{exp}) reveal increasing spacing with strain and large sample to sample variation.

Experimental vHs spacings as a function of θ_{int}, and tight binding predictions for several values of strain



Experiments show no correlation with small interlayer angle variation.

TB calculations including heterostrain show low influence of interlayer angle for a given strain.
On the contrary, a small variation of strain at a given angle has quite strong effect on the vHs spacing.

outlook

Identifying heterostrain as a critical parameter for this highly tunable system explains the ubiquitous sample to sample variability. Its implementation in the existing many models could be prolific. Yet, high variability remains when electron-electron interactions are strongest, pointing the need to renew the structural parametrization of flat band in that regime, when we know that combining heterostrain and twist angle is too simplistic. Sample environment is a good candidate because it can engineer the electrostatic environment that affects coulomb interactions and can also distort the flat bands through substate quality. Moreover, in STM experiments the tip can induce additional strain, locally modifying the relative stacking as well as the spacing between the two layers. This calls for a more systematic study of distorted flat bands, both in a local manner by the tip and by the substrate morphology and dielectric constant.

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