JULY 07, 2020
CONFERENCE ONLINE
Graphene Online &2DM Fundamental Research Insights
GO 2020

ELECTRONIC PROPERTIES of LOW-ANGLE TWISTED BILAYER GRAPHENE

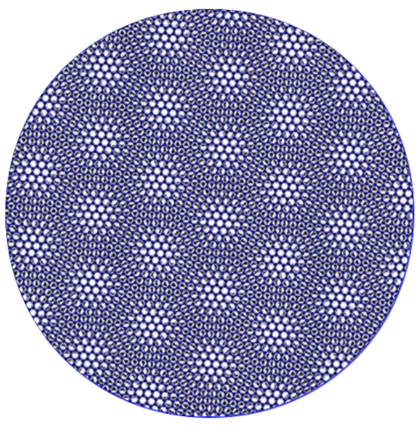
V.-H. Nguyen[1], D. Paszko[1] , B. van Troeye[2], M. Lamparski[2], V. Meunier[2], J.-C. Charlier[1]

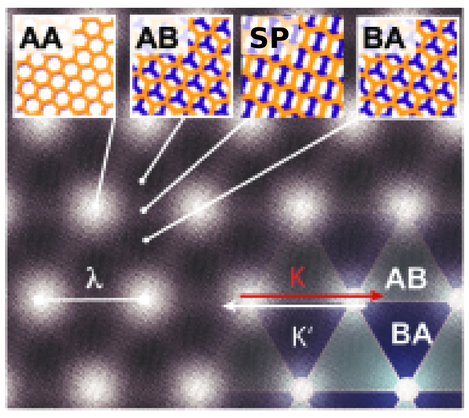
[1]Université Catholique de Louvain (UCLouvain), Louvain-la-Neuve, Belgium
[2]Rensselaer Polytechnic Institute, Troy, New York 12180, USA

Abstract: Twisted bilayer graphene is obtained by rotating one layer with respect to the other and is an important ingredient of the new field "twistronics" **[1]**. This system, generally forming moiré superlattices at large twist angles, however undergoes strong self-organized lattice reconstruction at low angles ($\lesssim 1°$), thus resulting in helical networks **[2]**. In this work, we investigate the electronic properties of low-angle twisted bilayer graphene using atomistic tight-binding calculations and taking into account the effects of such lattice reconstruction. It is shown that the lattice reconstruction represents strong effects on the electronic structure at low angles ($\lesssim 1°$), compared to those obtained at large angles ($> 1°$). By analyzing both global and local pictures, the electronic properties of these systems are systematically clarified.

Twisted bilayer graphene

Moiré superlattices ➡ Helical networks (e.g. see in **[2]**)



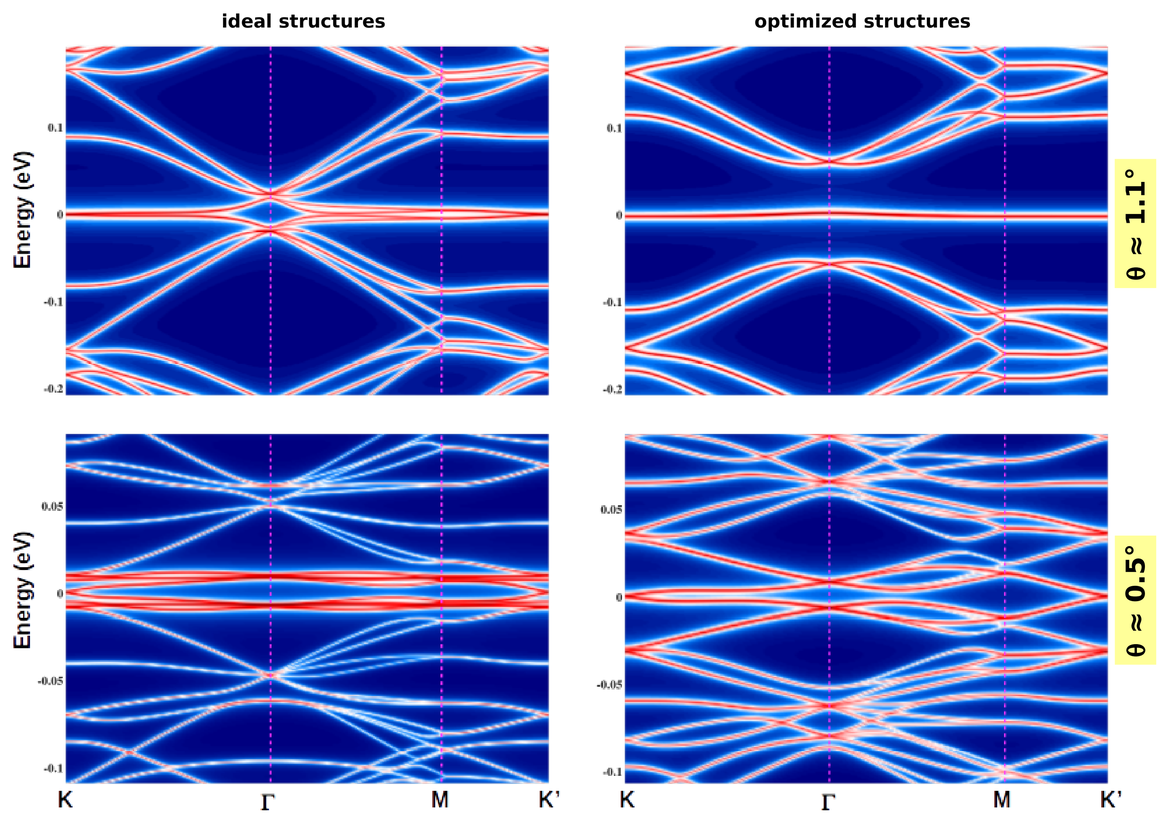


reduce twist angle ⟶

Calculation methodologies

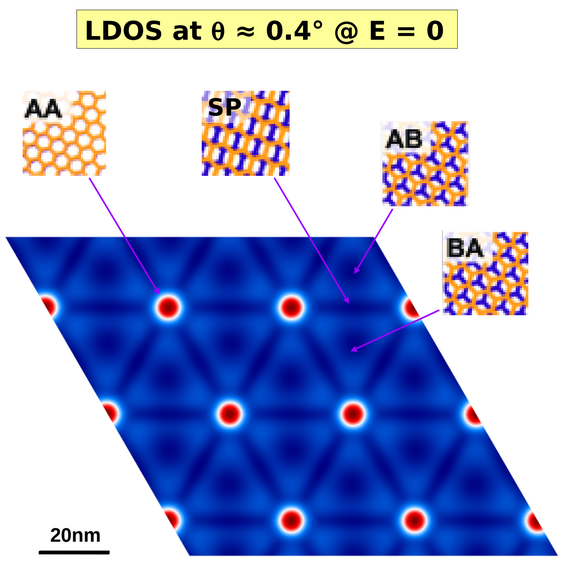
- structures are optimized using classical molecular dynamics simulations with interatomic potential models **[3]**
- electronic structure is modeled by the empirical tight-binding Hamiltonian presented in **[4]**
- electronic quantities are computed using recursive Green's function techniques **[5]**

Electronic bandstructure

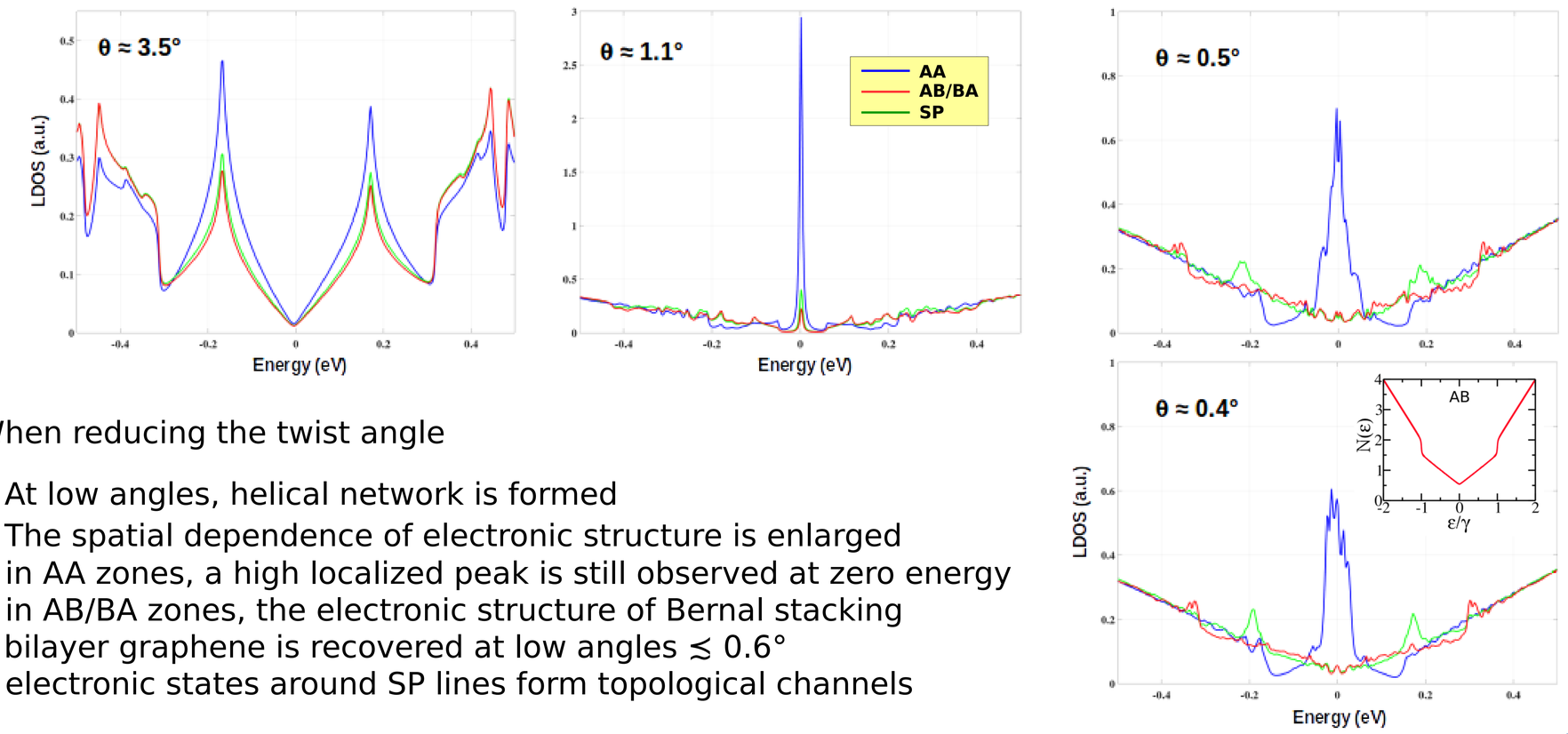


☒ The lattice reconstruction strongly affects the banstructure, especially, at low twist angles
☒ The second magic angle ~0.5° predicted in **[6]** is not observed

Local electronic properties



reduce twist angle ⟶



When reducing the twist angle

☒ At low angles, helical network is formed
☒ The spatial dependence of electronic structure is enlarged
- in AA zones, a high localized peak is still observed at zero energy
- in AB/BA zones, the electronic structure of Bernal stacking bilayer graphene is recovered at low angles $\lesssim 0.6°$
- electronic states around SP lines form topological channels

Summary: Electronic properties of low-angle twisted bilayer graphene taking into account the lattice reconstruction were systematically investigated **[7]**. The lattice reconstruction represents significant effects on the electronic structure at twist angles $\lesssim 1°$. In particular, whereas the flat bands at the first magic angle are conserved, the second magic angle ~0.5° predicted in **[6]** is no longer observed. This is a direct consequence of the strong lattice reconstruction at low twist angles. Actually, when the twist angle is small enough (i.e., $\lesssim 0.6°$), the AB zones are large and thus locally present the well-known electronic structure of Bernal stacking bilayer graphene. In addition, the AB zones and accordingly their contribution to the global electronic properties of the system are significantly enlarged when reducing the twist angle. This explains essentially our obtained results showing that whereas a zero-energy localized peak of LDOS is still observed in the AA zones, such peak (accordingly flat bands) is smeared out and then disappears in the total DOS of the system at low angles << 1°.

CONTACT

viet-hung.nguyen@uclouvain.be

REFERENCES

[1] A. H. MacDonald, Physics **12** (2019) 12; **[2]** Peter Rickhaus ***et al.***, Nano Lett. **18** (2018) 6725-6730; Hyobin Yoo ***et al.***, Nat. Mater. **18** (2019) 448–453; **[3]** M. Lamparski, B. Van Troeye and V. Meunier, 2D Materials **7** (2020) 025050; **[4]** Andreij C. Gadelha ***et al.***, arXiv:2006.09482; **[5]** G. Thorgilsson ***et al.***, J. Comp. Phys. **261** (2014) 256-266; **[6]** R. Bistritzer and A. H. MacDonald, PNAS **108** (2011) 12233-12237; **[7]** D. Paszko ***et al.***, in preparation

Graphene Online &2DM Fundamental Research Insights
GO 2020