

Structural and electronic properties of twisted MoS₂ bilayers

Somepalli Venkateswarlu

Andreas Honecker, Guy Trambly de Laissardière.

Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), CY Cergy Paris Université, 95302 Cergy-Pontoise, France .

somepalli.venkateswarlu@u-cergy.fr

Vertically stacked transition metal dichalcogenides of multilayer structures have gained increasing attention because of their fascinating features in electronics and optical properties [1]. We performed the calculation of structural and electronic properties of twisted MoS₂ bilayers using first principle calculations (ABINIT [2]) and Tight-binding method (TB). The result shows that significant differences in the band structures of twisted and non-twisted ones: the appearances of the crossover between direct and indirect bandgap, gap variation and atomic relaxations. For rather large rotation angles Θ between the two layers, the band structures with different Θ are very similar [3]. For the smallest angles, the stacking forms a Moiré pattern (figure 1) and TB calculations predict some flat bands in the valence band and the conduction band. As in twisted bilayer graphene, those states are localized in the AA stacking region of the Moiré as shown by the fine peaks in the local density of states (figure 2).

References

- [1] E. S. Kadantsev, P. Hawrylak, Solid State Comm. **152** (2012) 909
- [2] X. Gonze et al., Comp. Mat. Sci. **25** (2002) 478. <https://www.abinit.org>
- [3] Z. Wang et al., J. Phys. Chem. C , **119** (2015) 4752-4758

Figures :

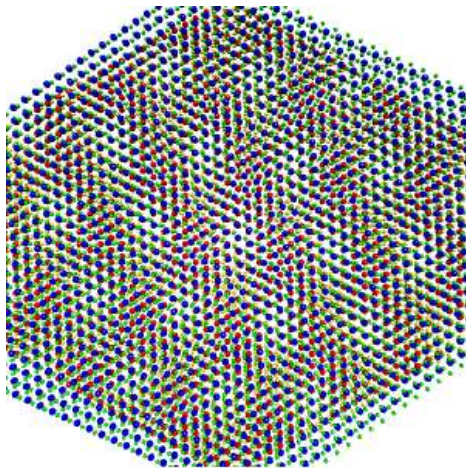


Figure 1: Moiré pattern of twisted MoS₂ bilayers [5.08°] & color indicates Top layer [Blue (Molybdenum (Mo)), Green (Sulphur (S))], Bottom layer [Red (Molybdenum (Mo)), Yellow (Sulphur (S))].

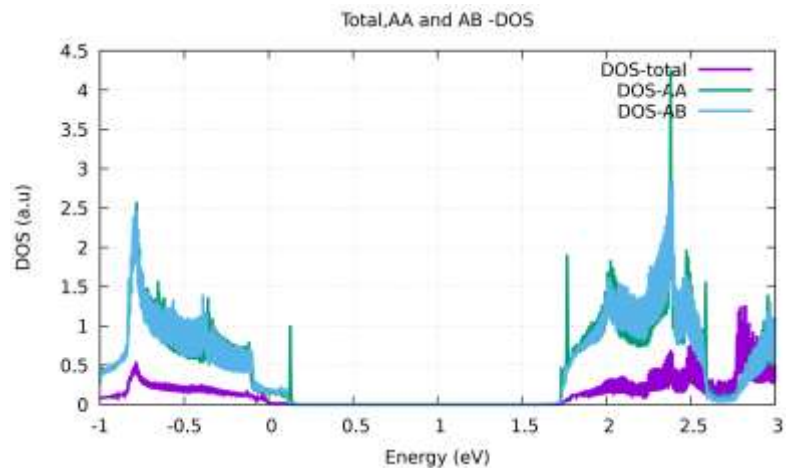


Figure 2: Local electronic density of states (DOS) of twisted MoS₂ bilayer with rotation angle 1.27°: (DOS-AA) Local DOS on Mo d_{z²} orbital at the center of AA stacking region, (DOS-AB) local DOS on Mo d_{z²} orbital at the center of AB stacking region, (DOS-total) total DOS.