Electronic localization in twisted bilayer MoS$_2$ with small rotation angle.

Venkateswarlu Somepalli

Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université /CNRS, F-95302 Cergy-Pontoise, France

Dr. Guy Trambly de Laissardières

Prof. Dr. Andreas Honecker
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**MoS\textsubscript{2} monolayer:**

- DFT based first principle calculation were carried out using ABINIT software program.
  - X. Gonze et al, Computer Physics Communications. **205**, 106-131 (2016).

**MoS\textsubscript{2} lattice structure.** Blue circles represent Mo atoms & yellow circles represent S atoms.

- Monolayer \textit{MoS}\textsubscript{2} \quad Direct band gap ≈ 1.7 to 1.9 eV
- Bulk \textit{MoS}\textsubscript{2} \quad In direct band gap ≈ 1.2 eV

**Electronic band structure of MoS\textsubscript{2} monolayer (DFT).**

- Good agreement with previous calculations.
  - E. S. Kadantsev, Solid State Communications **152**, 909–913 (2012).
  - O. Lopez-Sanchez, et al., Nature Nanotech, (2013).
  - M. Kan et al, \textit{J. Phys. Chem. C} **118**, 3, 1515-1522 (2014).
Atomic structure of twisted MoS$_2$ bilayer:

\[ \cos \theta = \frac{n^2 + 4nm + m^2}{2(n^2 + nm + m^2)} \]

\[ N=6(n^2+nm+m^2) \]

- Fig. Atomic structure of bilayer MoS$_2$ at a twist angle (n=2, m=3)
  \[ \theta = 13.17^\circ \].
  (a) sideview. (b) top view.

arXiv:2005.13054.
Electronic band structure of twisted MoS$_2$ bilayer with different angles:

- DFT electronic band structure of twisted bilayer of MoS$_2$ : (n=1, m=2) $\theta = 21.79^\circ$, (n=2, m=3) $\theta = 13.17^\circ$, (n=3, m=4) $\theta = 9.43^\circ$, & (n=4, m=5) $\theta = 7.34^\circ$. For every rotation angle, the origin of energy is fixed at the energy of the state $S_0$.

arXiv:2005.13054.
Tight-binding Model:

Tight-Binding model parameters

Onsite energies of D and P orbitals (eV)

| Orbital                   | Energy (eV) |
|---------------------------|-------------|
| D0 (d3z2-r2)              | 0.1356      |
| D1 (dyz, dzx)             | -0.4204     |
| D2 (dxy, dx2-y2)          | 0.0149      |
| DP (Px, Py)               | -38.71      |
| Dz (Pz)                   | -29.45      |

Slater-Koster parameters (Intralayer) (eV)

| Parameter | Energy (eV) |
|-----------|-------------|
| Vddπ      | 0.7027      |
| Vddσ      | -0.9035     |
| Vddδ      | 0.0897      |
| Vppπ      | -2.678      |
| Vppσ      | 8.079       |
| Vpdπ = Vdpπ | 3.267   |
| Vpdσ = Vdsn | -7.193   |

Tight-Binding Hamiltonian for independent electrons.

\[ H = \sum_i \epsilon_i |i><i| + \sum_{i,j} t_{ij} |i><j| \]

Adapted from E Ridolfi et al, J. Phys. Condens. Matter 27 365501 (2015). R. Roldán et al, Appl. Sci. 6, 284 (2016). . . .
Electronic band structure of MoS$_2$ mono layer (DFT+TB):

➢ Our Tight binding model parameters are good agreement with first principle calculations [ABINIT] of mono layer of MoS$_2$ electronic band structure, around the bandgap region.

arXiv:2005.13054.
Tight-binding Model:

\[ V = V_0 e^{q \left(1 - \frac{d}{d_{min}}\right)} \]

| Slater-Koster parameters (Interlayer) Mo (d) – Mo (d). |\n| \hline | \hline | \hline |
| Vddπ | V (eV) | q | d_{min}(Å) |
| -0.4254 | 11.6496 | 2.1384 |
| Vddσ | -0.1416 | 11.6496 | 2.1384 |
| Vddδ | -0.1237 | 11.6496 | 2.1384 |

| Slater-Koster parameters (Interlayer) S (p) – S (p). |\n| \hline | \hline | \hline |
| Vddπ | -8.9733 | 6.2981 | 1.5606 |
| Vddσ | 6.2782 | 6.2981 | 1.5606 |

| Slater-Koster parameters (Interlayer) S (p) – Mo (d). |\n| \hline | \hline | \hline |
| Vpdπ = Vdπp | 0.5243 | 8.9738 | 1.6472 |
| Vpdσ = Vdσp | -1.4793 | 8.9738 | 1.6472 |

arXiv:2005.13054.
Electronic band structure of twisted MoS$_2$ bilayer (DFT+TB): 

(n=1, m=2) $\theta = 21.79^\circ$. 

(n=3, m=4) $\theta = 9.43^\circ$. 

arXiv:2005.13054.
Analysis  band of twisted bilayer of MoS$_2$ (built from AA-stacking):

**Fig:** Dependence of valence bands on rotation angle $\theta$:

(a) Valence band dispersion of (n=4, m=5) tb- MoS$_2$, $\theta = 7.43^\circ$.

(b) Energy $E(S_2)$ of the state $S_2$ (see panel (a)) versus $\Theta^2$.

(c) Energy difference between the states $S_4$ and $S_2$,

$\Delta E_{24} = E(S_4) - E(S_2)$, versus $\theta$. A negative value of $\Delta E_{24}$ means that a gap $|\Delta E_{24}|$ exists between the band below the gap and the other valence bands.

(d) Average slope of $E(k)$ of the band between states $S_2$ and $S_3$.

arXiv:2005.13054.
Moiré pattern of twisted bilayer of MoS$_2$:

Fig: Atomic structure of (n=6, m=7) $\theta = 5.09^\circ$ tb-MoS$_2$ built from AA-stacked bilayers. Black lines show the unit cell. AA stacking regions are at the corners of this cell, BA’ and AB’ staking regions are at 1/3 and 2/3 of its longest diagonal, respectively.

arXiv:2005.13054.
Local density of states (LDOS) of twisted bilayer of MoS$_2$:

**Fig:** LDOS of the Mo orbital around the main gap in (n=6, m=7) tb- MoS$_2$, $\theta = 5.09^\circ$ (Built from AA-stacking):

LDOS of $d_0 = 4d_z^2$, $d_1 = 4d_{xz}$, $4d_{yz}$ and $d_2 = 4d_x^2 - d_y^2$, $4d_{xy}$ Mo orbitals at the centre of the AA stacking region.

The LDOS is calculated employing a Gaussian broadening with the standard deviation $\sigma = 2$ meV. arXiv:2005.13054.
Confined state in the AA-region of moiré pattern of twisted bilayer of MoS$_2$:

In a moiré cell, two symmetrically equivalent AB stacking regions are located at 1/3 and 2/3 of the diagonal of the cell. Each AB stacking region contains two types of Mo atoms: (AB-A) Mo atom of a layer lying above an S atom of the other layer; (AB-B) Mo atom of a layer not lying above an atom of the other layer. 

Fig: Tb band dispersion and local density of states (LDOS) of $d_0 = d_z^2$ Mo atoms at the centre of the AA-stacking region and the centre of the AB-region: 

(a) (n=20, m=21) tb-MoS$_2$, $\theta = 1.61^\circ$. 

arXiv:2005.13054.
Eigenstates corresponding to flat bands in twisted bilayer of MoS$_2$:

**Fig:** Average weight of the eigenstates at $\Gamma$, $K$, and $M$ of the flat bands around the gap in real space in (20, 21) tb- MoS$_2$ $\theta = 1.61^\circ$ (built from AA-stacking):

Conduction band:
(a) Average of the four-fold quasi-degenerate band at energy $E \approx 1.686 \pm 0.002$ eV.
(b) Average of the two-fold quasi-degenerate band at energy $E \approx 1.6626 \pm 0.0002$ eV.

Valance band:
(c) Non-degenerate band at energy $E \approx 0.26249 \pm 0.00001$ eV.
(d) Average of the two-fold quasi-degenerate band at energy $E \approx 0.2518 \pm 0.0003$ eV.

arXiv:2005.13054.
Conclusion:

✓ We have revisited the tight-binding description of twisted MoS$_2$ bilayers starting from DFT computations.
✓ We found that isolated bands appear in the valence and conduction bands close to the gap for $\theta \leq 5$-$6^\circ$.
✓ For very small angles $\theta \leq 2^\circ$, the average velocity vanishes.
✓ Depending on the flat band, this real space confinement occurs at the centre of the AA region and also in a ring around the centre of the AA region.
✓ We checked AB-stacking and different Tb-models, qualitatively same behaviour.

❖ Correlation effects in twisted-bilayer of MoS$_2$.
❖ Quantum transport properties of twisted-bilayer of MoS$_2$.
Thank you for your attention.