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

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DFT calculations:
• Electronic band structure of twisted bilayer of MoS$_2$ with different angles.

TB calculations:
• Monolayer of MoS$_2$.
• Twisted bilayer of MoS$_2$ (tb- MoS$_2$).
• Analysis of band of tb- MoS$_2$ (built from AA-stacking).
• Moiré pattern of tb- MoS$_2$
• Local density of states.
  ➤ Confined state in the AA region of moiré pattern.
• Eigenstates corresponding to flat bands in tb- MoS$_2$.

Conclusion.
MoS$_2$ 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$_2$ lattice structure. Blue circles represent Mo atoms & yellow circles represent S atoms.

Monolayer MoS$_2$  Direct band gap ≈ 1.7 to 1.9 eV

Bulk MoS$_2$  In direct band gap ≈ 1.2 eV

Good agreement with previous calculations.

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.

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 $S_0$.

Tight-binding Model:

Tight-Binding model parameters

<table>
<thead>
<tr>
<th>Onsite energies of D and P orbitals (eV)</th>
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<tr>
<td>D0 ( (d_{3z^2-r^2}) )</td>
<td>0.1356</td>
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<tr>
<td>D1 ( (d_{yz}, d_{zx}) )</td>
<td>-0.4204</td>
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<td>D2 ( (d_{xy}, d_{x^2-y^2}) )</td>
<td>0.0149</td>
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<td>DP ( (P_x, P_y) )</td>
<td>-38.71</td>
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<td>Dz ( (P_z) )</td>
<td>-29.45</td>
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Slater-Koster parameters (Intralayer) (eV)

| Vddπ                  | 0.7027     |
| Vddσ                  | -0.9035    |
| Vddδ                  | 0.0897     |
| Vppπ                  | -2.678     |
| Vppσ                  | 8.079      |
| Vpdπ = Vdpπ           | 3.267      |
| Vpdσ = Vdpσ           | -7.193     |

\[
\begin{align*}
H &= \sum_i \epsilon_i |i><i| + \sum_{(i,j)} t_{ij} |i><j|
\end{align*}
\]


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.

Tight-binding Model:

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

<table>
<thead>
<tr>
<th>Slater-Koster parameters (Interlayer) Mo (d) – Mo (d).</th>
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<tr>
<td>( Vdd\pi )</td>
<td>( V ) (eV)</td>
<td>( q )</td>
<td>( d_{\text{min}} ) (Å)</td>
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<tr>
<td>-0.4254</td>
<td>11.6496</td>
<td>2.1384</td>
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<td>( Vdd\sigma )</td>
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<td>( Vdd\delta )</td>
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<tr>
<td>( Vdd\pi )</td>
<td>-8.9733</td>
<td>6.2981</td>
<td>1.5606</td>
</tr>
<tr>
<td>( Vdd\sigma )</td>
<td>6.2782</td>
<td>6.2981</td>
<td>1.5606</td>
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<tbody>
<tr>
<td>( Vp\delta\pi = Vd\rho\pi )</td>
<td>0.5243</td>
<td>8.9738</td>
<td>1.6472</td>
</tr>
<tr>
<td>( Vp\delta\sigma = Vd\rho\sigma )</td>
<td>-1.4793</td>
<td>8.9738</td>
<td>1.6472</td>
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</table>

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

(n=1, m=2) $\theta = 21.79^\circ$.  
(n=3, m=4) $\theta = 9.43^\circ$.

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 $S_3$.

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' stacking regions are at 1/3 and 2/3, of its longest diagonal, respectively.

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. 
Confined state in the AA-region of moiré pattern of twisted bilayer of MoS$_2$:

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$_2$, $\theta = 1.61^\circ$.

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.

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.

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 $\theta \leq 5\text{-}6^\circ$.
✓ 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.