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Electronic localization in twisted bilayer MoS_2 with small rotation angle.

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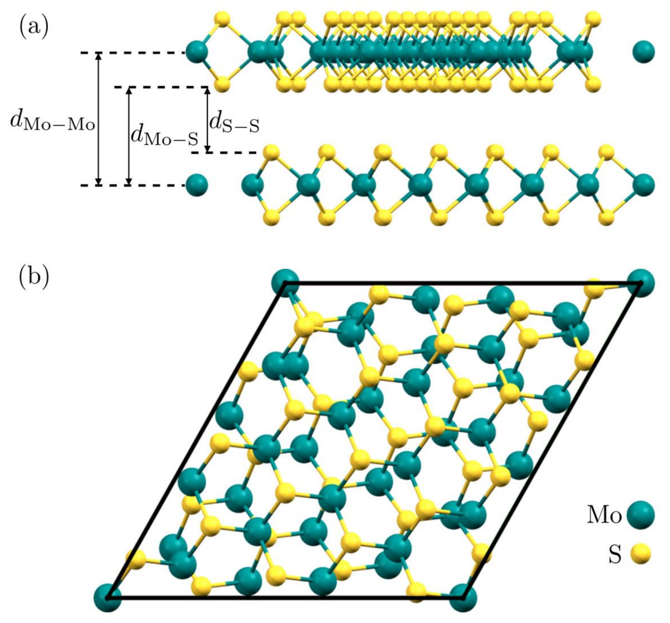
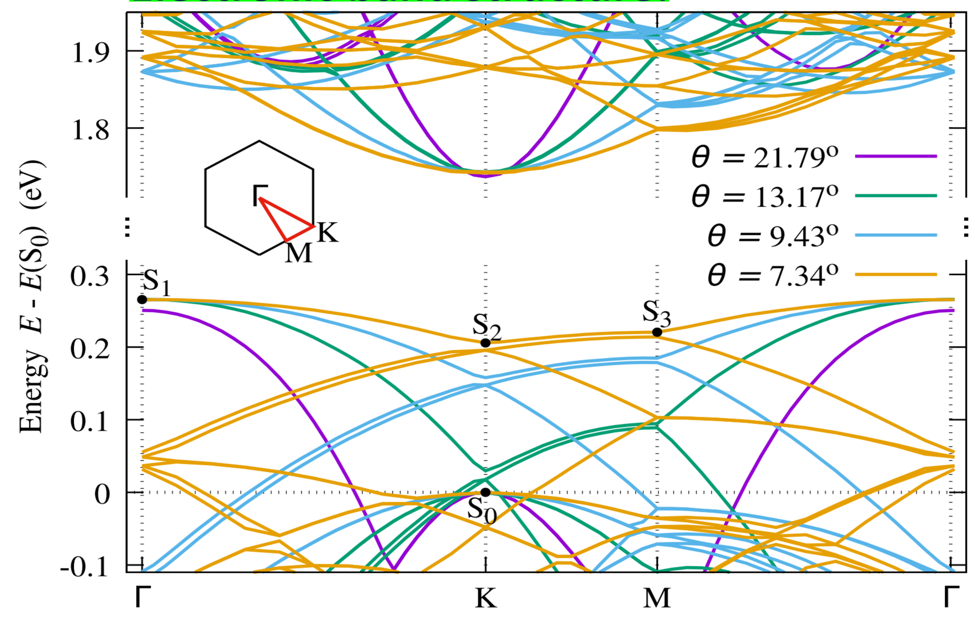
ABSTRACT: Moiré patterns are known to confine electronic states in transition metal dichalcogenide bilayers, thus generalizing the notion of magic angles discovered in twisted bilayer graphene to semiconductors. Here, we present a revised Slater-Koster tight-binding model that facilitates reliable and systematic studies of such states in twisted bilayer MoS_2 for the whole range of rotation angles θ. We show that isolated bands appear at low energy for $\theta \leq 5°$– 6°. Moreover, these bands become "flatbands," characterized by a vanishing average velocity, for the smallest angles $\theta \leq 2°$ [1].

Twisted MoS_2 bilayer:

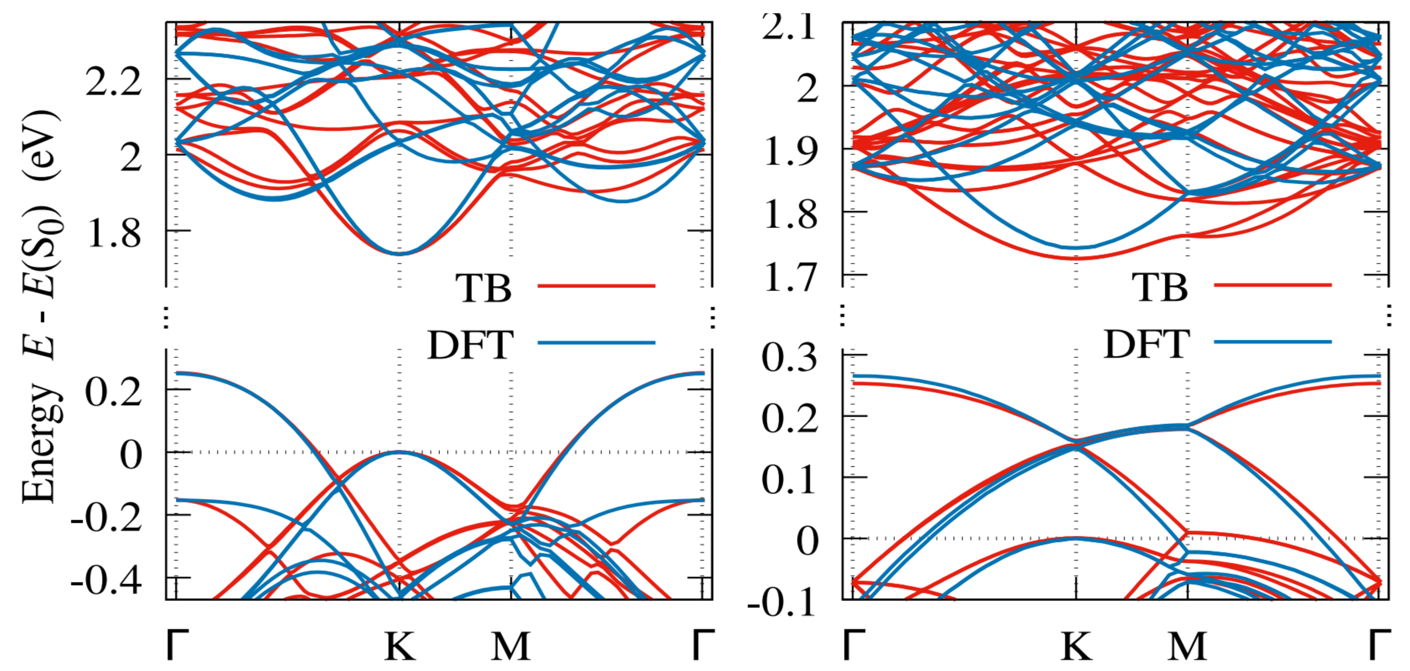


Atomic structure of bilayer MoS_2 at a twist angle θ = 13.17°. (a) Side view. (b) Top view [1].

Electronic band structure:



DFT conduction and valence bands in tb- MoS_2 : (1, 2) θ = 21.79°, (2, 3) θ = 13.17°, (3, 4) θ = 9.43°, and (4, 5) θ = 7.34°. For every rotation angle, the origin of energy is fixed at the energy of the state S_0 [1].



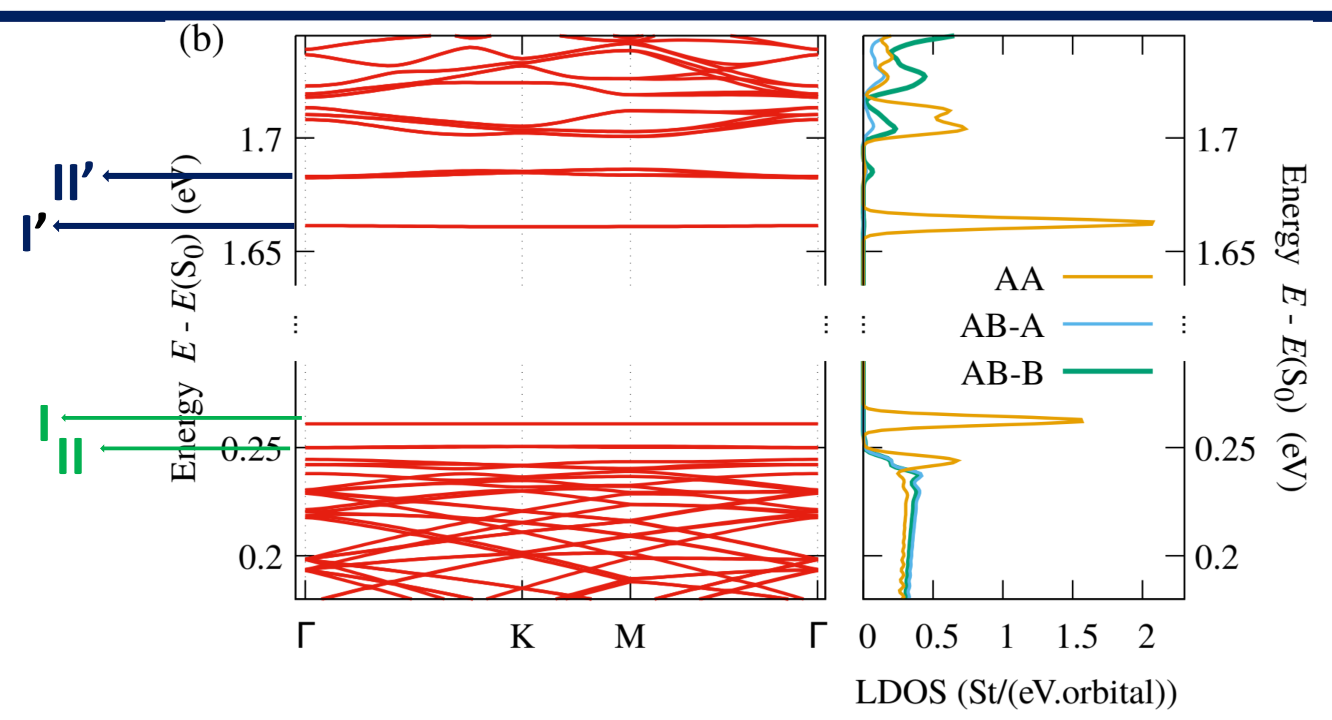
TB and DFT bands around the gap in tb-MoS2: (left)(1, 2) θ = 21.79° and (right) (3, 4) θ = 9.43° [1].

METHODOLOGY:

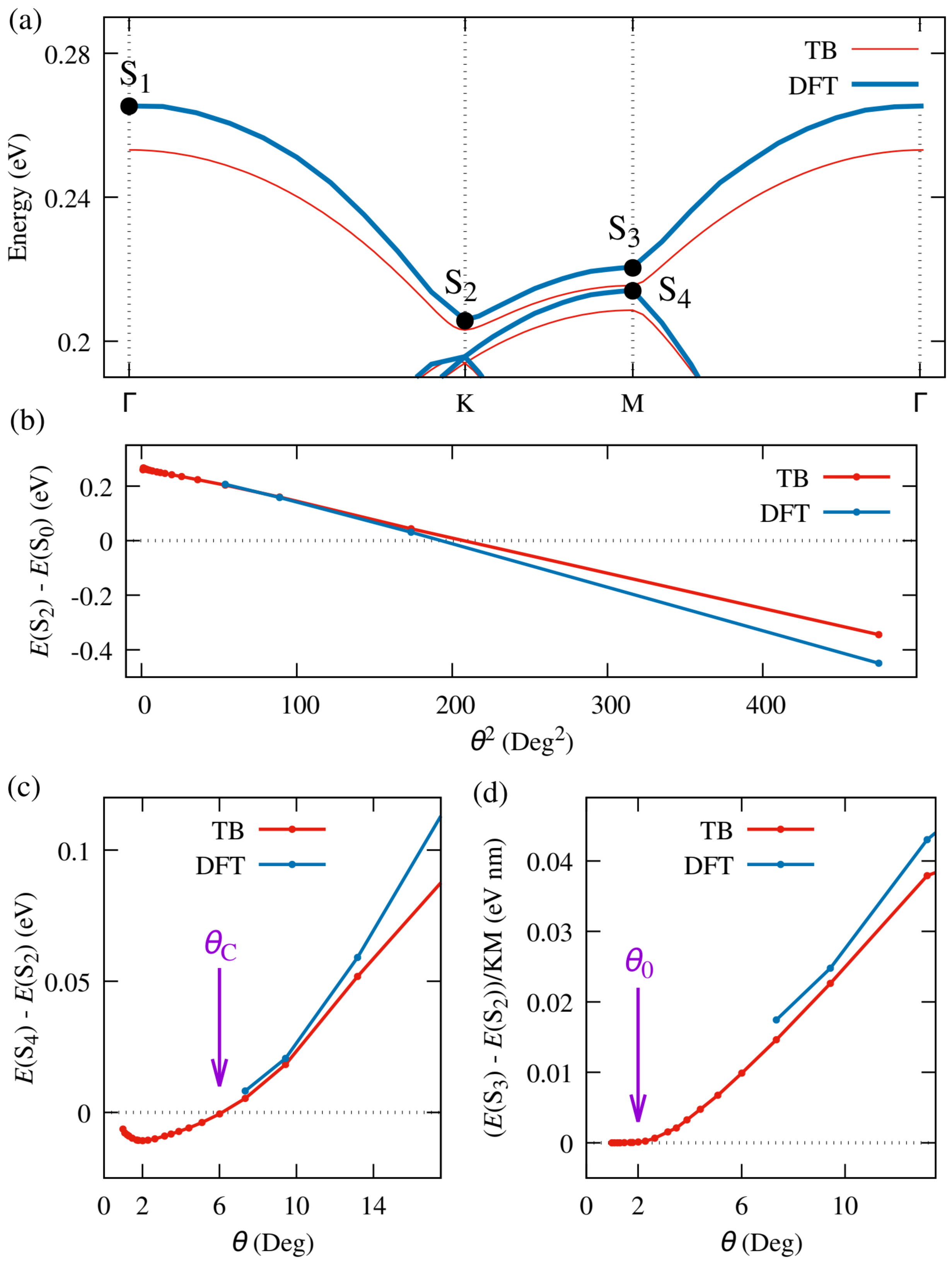
- ✓ ABINIT [3] is the software that was employed to carry out the DFT calculations. Different pseudopotentials [GGA and LDA].
- ✓ Tight Binding Model (TB) [1, 2], in the unit cell 5-d orbitals of Mo atom & 6-p orbitals of two S atoms.

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{\langle i,j\rangle} t_{ij} |i\rangle\langle j| \qquad \cos\theta = \frac{n^2+4nm+m^2}{2(n^2+nm+m^2)}$$

- ✓ Electronic quantities are computed using Gaussian broadening (DOS) method and exact diagonalization method [1].



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: (b) (n=20, m=21) tb-MoS_2, θ = 1.61 [1].



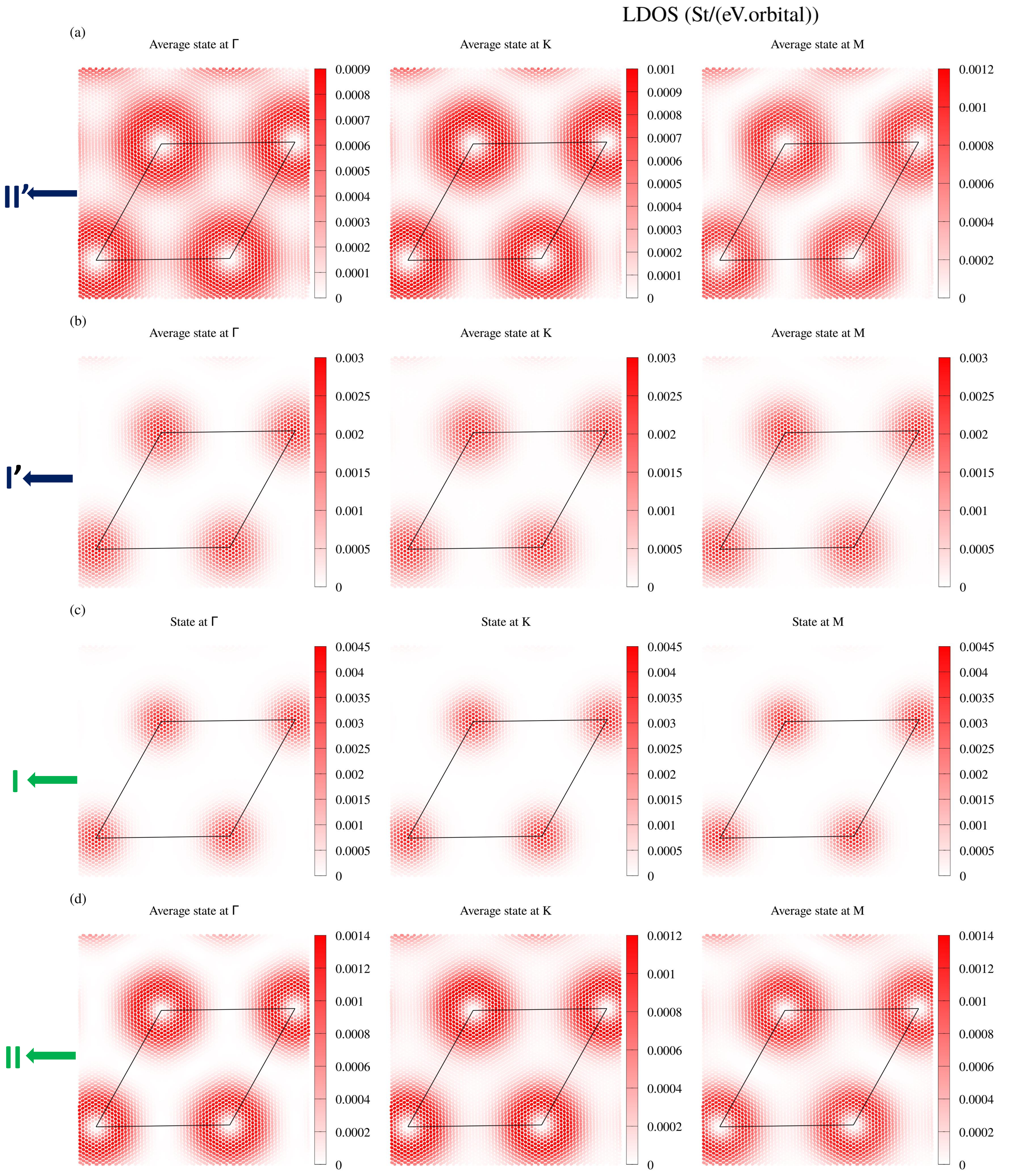
Dependence of valence bands on rotation angle θ [1] :

(a) Valence band dispersion of (n=4, m=5) tb- MoS_2, θ = 7.43°.

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

(c) Energy difference between the states S_4 and S_2, $\Delta E_{24} = E(S_4)-E(S_2)$, versus θ . A negative value of ΔE_{24} means that a gap | ΔE_{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.



Average weight of the eigenstates at Γ, K, and M of the flat bands around the gap in real space in (20, 21) tb- MoS_2 θ = 1.61° (built from AA-stacking) :

Conduction band:

(a) Average of the four-fold quasi-degenerate band at energy E ≈ 1.686 ± 0.002 eV.

(b)Average of the two-fold quasi-degenerate band at energy E ≈ 1.6626 ± 0.0002 eV.

Valance band:

(c) Non-degenerate band at energy E ≈ 0.26249 ± 0.00001 eV.

(d) Average of the two-fold quasi-degenerate band at energy E ≈ 0.2518 ± 0.0003 eV [1] .

SUMMARY: We found that isolated bands appear in the valence and conduction bands close to the gap for θ ≤ 5°–6°. For even smaller angles θ ≤ 2°, the average velocity vanishes. The emergence of the corresponding flatbands is reflected by sharp peaks in the density of states. This phenomenon is accompanied by a localization of the wave function mainly in AA stacking regions. Depending on the flatband, this real-space confinement can occur at the center of the AA region and also in a ring around the center of the AA region. In the present discussion, we have focused on rotated MoS_2 bilayers that are constructed from AA stacking, but we have checked [1] that qualitatively the same behavior is found when one starts from AB stacking instead. The vanishing velocity and related emergence of flatbands identifies weakly doped MoS_2 bilayers as good candidates for the observation of strong correlation effects. Beyond first theoretical efforts in this direction [4], we offer our DFT-based tight-binding model as a solid starting point for more detailed studies of correlation effects in twisted MoS2 bilayers [1].

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