Flat bands in twisted bilayer transition metal dichalcogenides.

Manish Jain

Centre for Condensed Matter Theory,
Department of Physics,
Indian Institute of Science,
Bangalore

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Novel Phases of Quantum Matter
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Motivation

- Recent interest in 'Magic angles' in twisted bilayer graphene [1].

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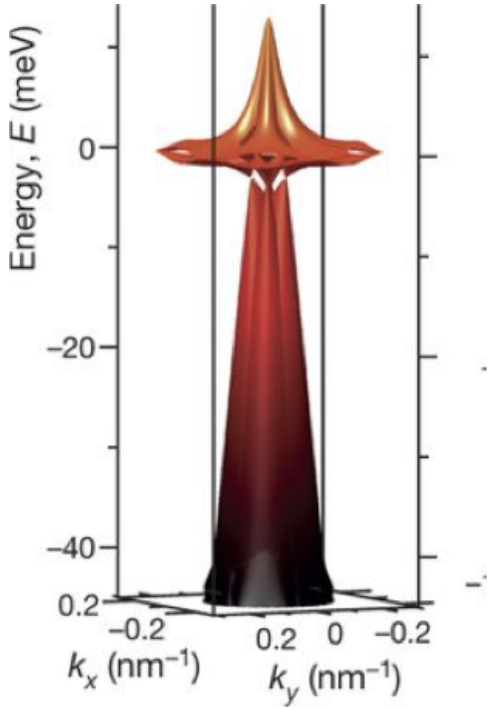

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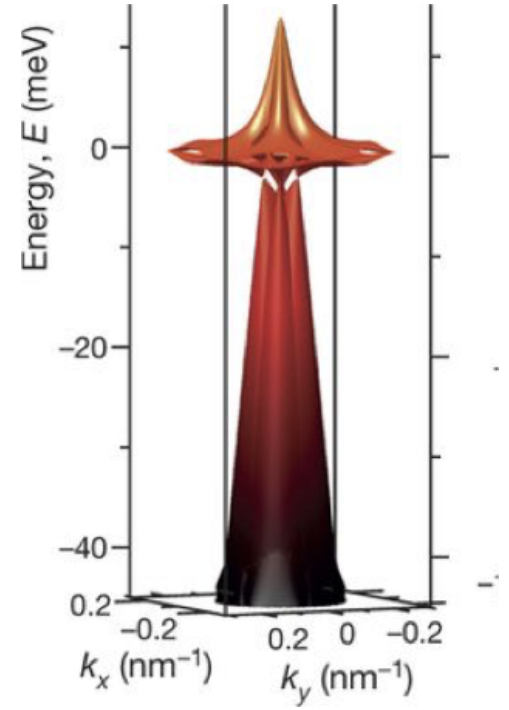

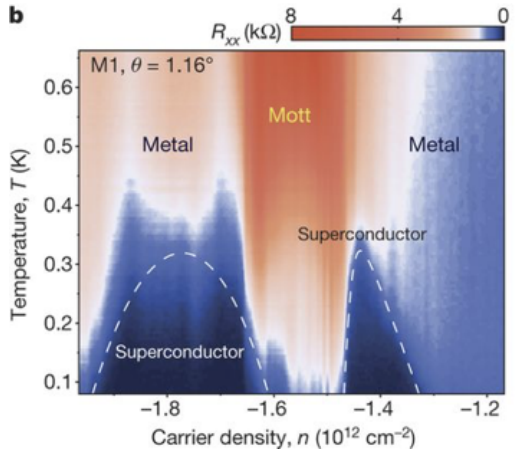

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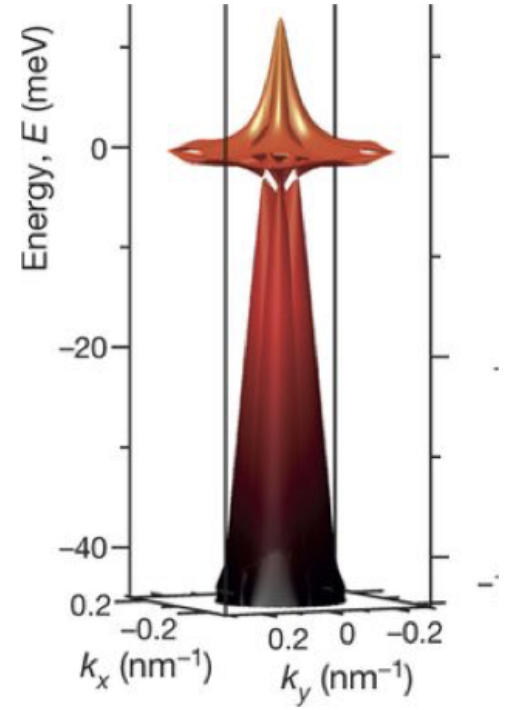

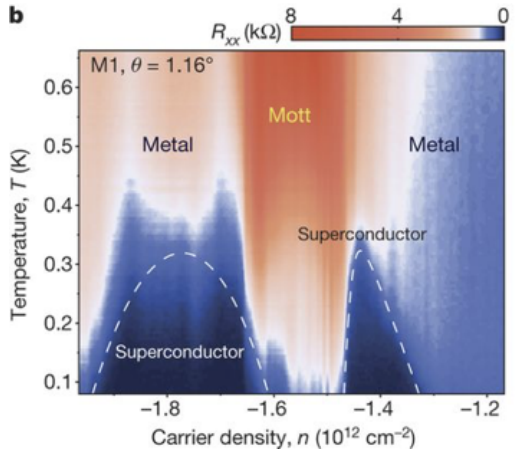

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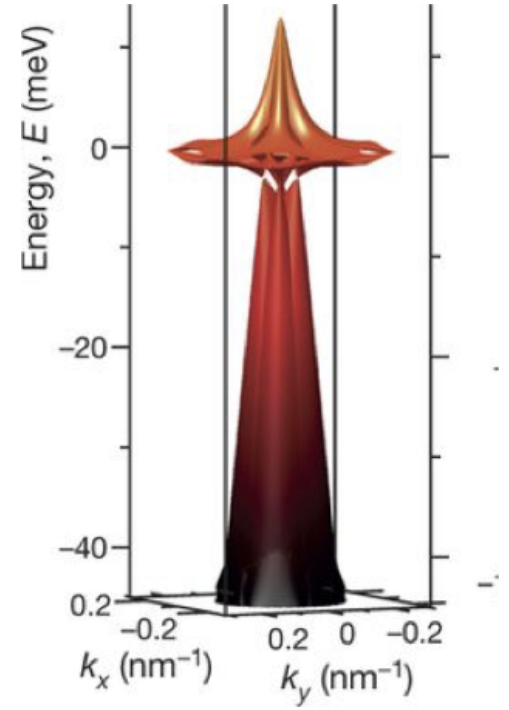
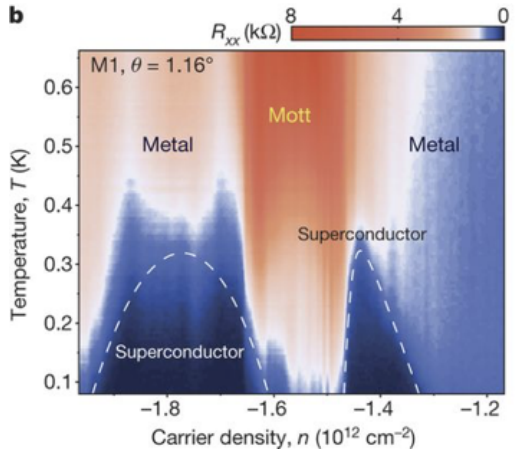
- Twisted bilayer transition metal dichalcogenides (TMDs) show similar flat bands [3].
- What is the origin of these flat bands in twisted bilayer TMDs?





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- Introducing a small-angle twist between the two layers of bilayer MoS_2 leads to the formation of a Moiré pattern.
- We study these Moire patterns for twist angles close to 0° and 60°.
- A geometrically commensurate superlattice is generated for each angle using the Twister code [1].

1. `http://www.physics.iisc.ernet.in/~mjain/software.html`

Computational Details – Multiscale approach

- DFT calculations for the larger angles[1] are performed using Quantum Espresso.
- Smaller angles contain too many atoms.
- Use *ab initio* calculations to parametrize Kolmogorov-Crespi Force-fields[2] for relaxation.
- Use SIESTA code for the electronic structure.

Angle	Atoms
5.1, 54.9	762
3.5, 56.5	1626
2.6, 57.4	2814
2, 58	5514
1.5, 58.5	8322

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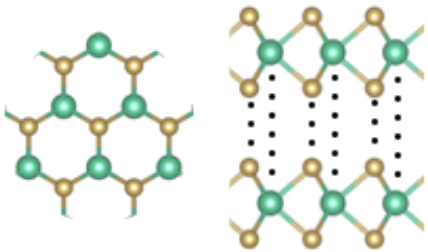
2. Mit H. Naik, Indrajit Maity, Prabal K. Maiti and Manish Jain, J. Phys. Chem. C **123** 9770-9778 (2019).

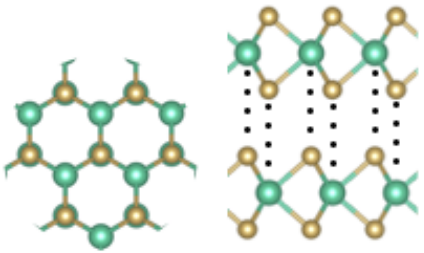
Stackings in BLM

Five unique high-symmetry stackings.

AA



AB



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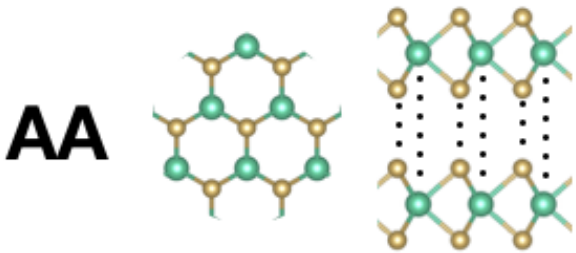

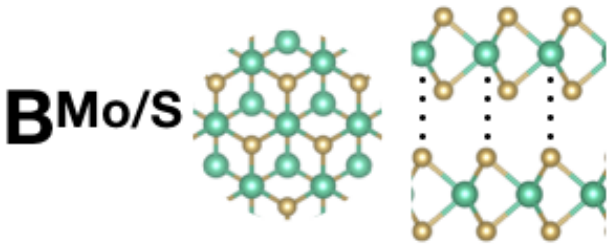

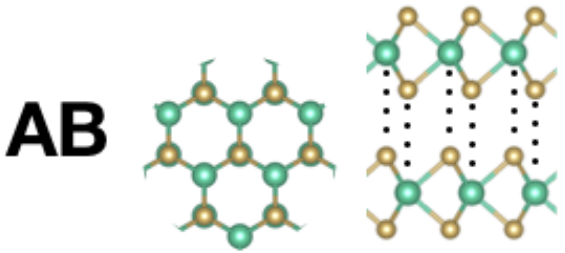

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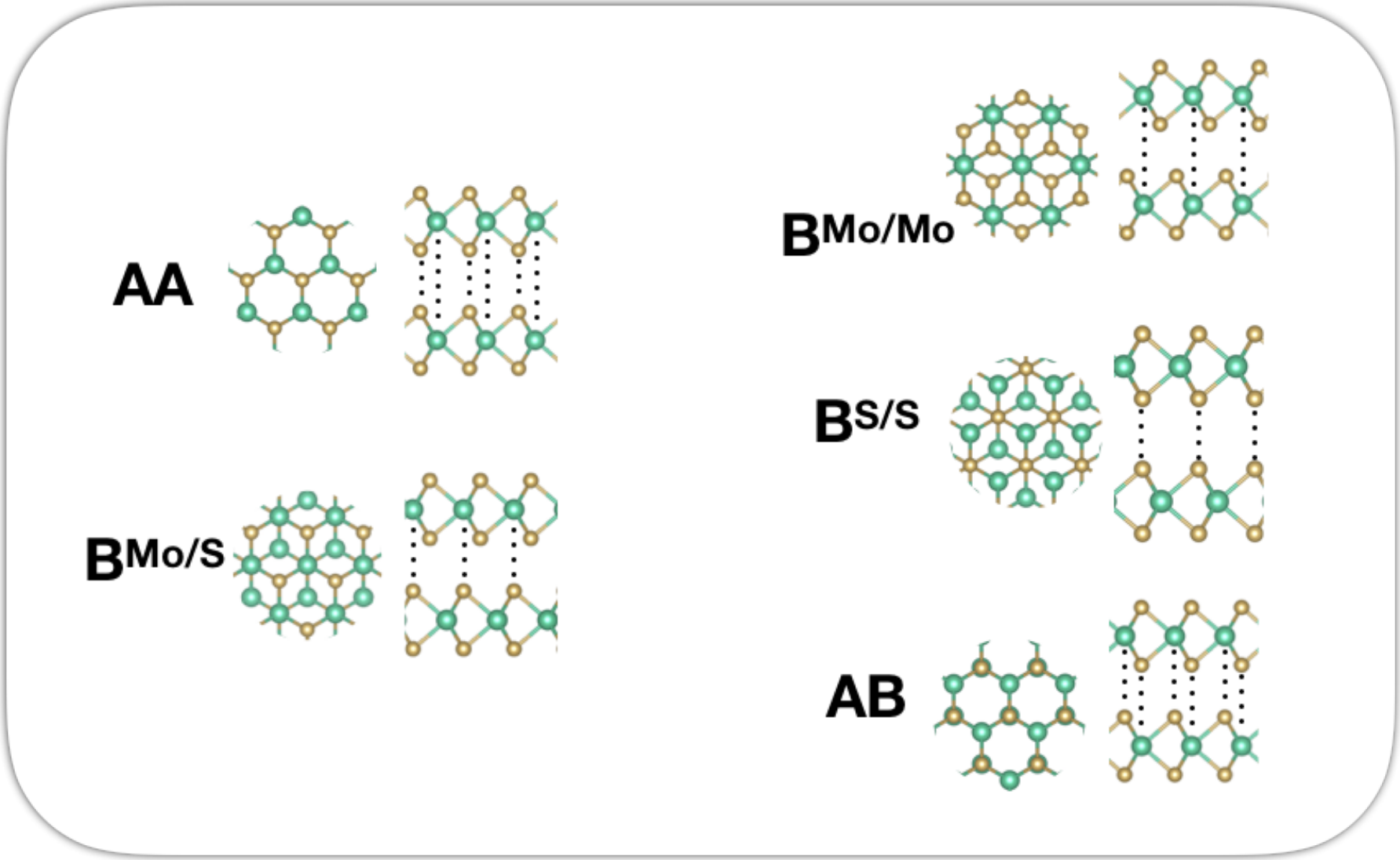
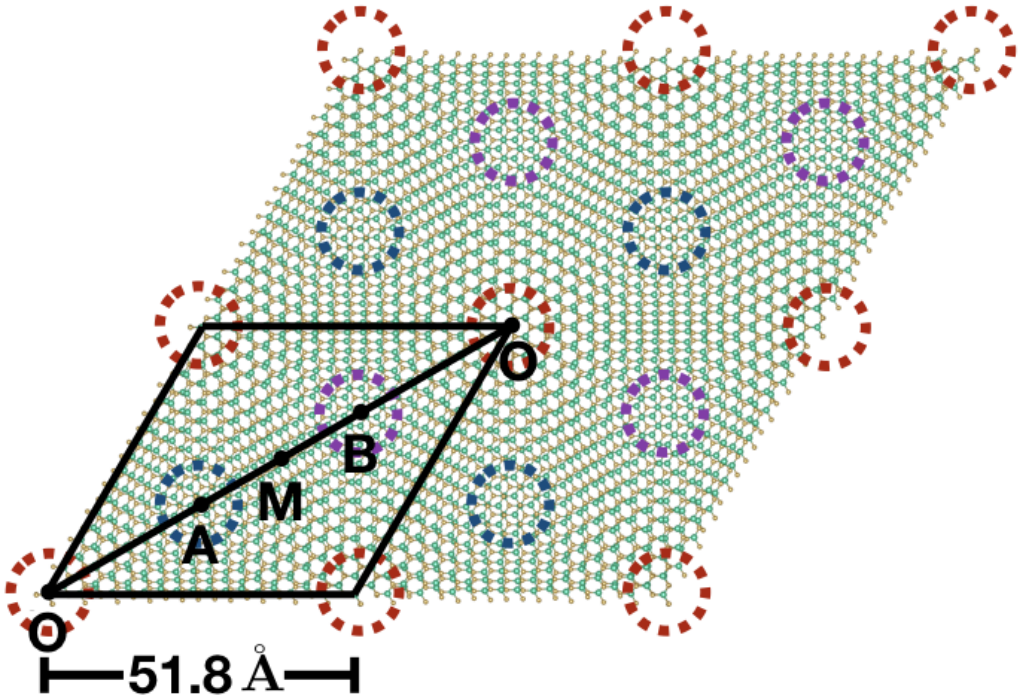
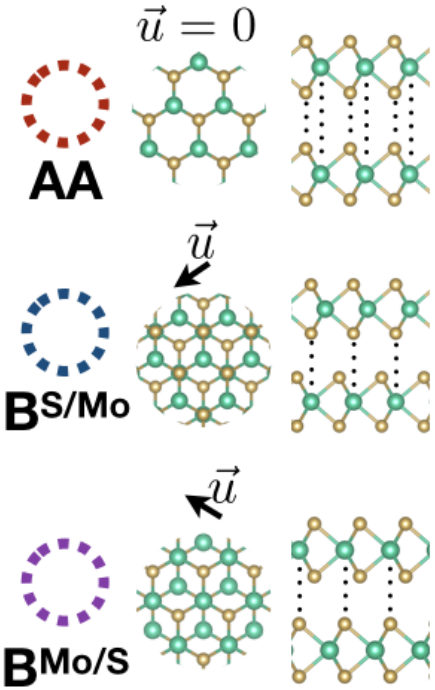


3.5° twist angle, $M^{3.5}$





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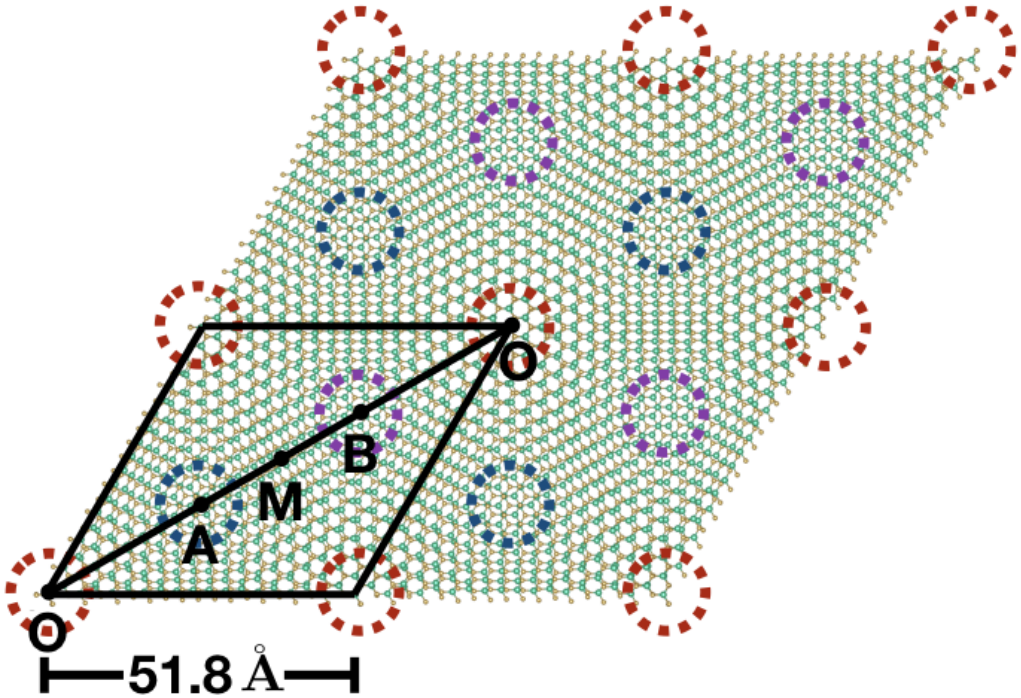

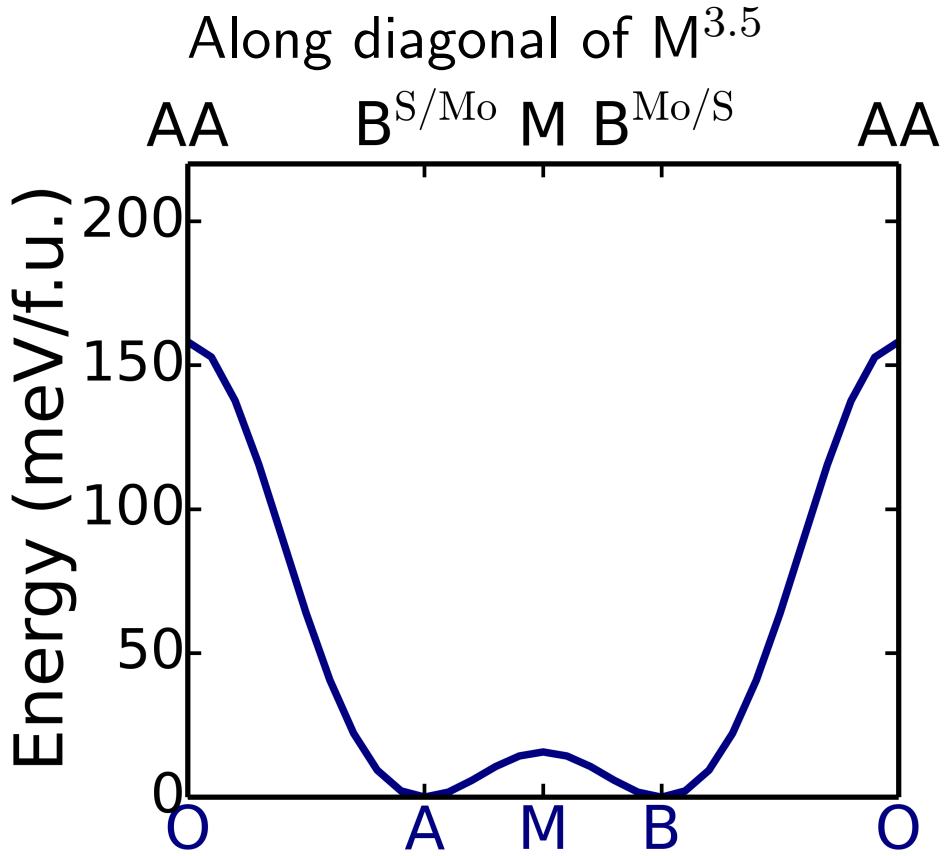

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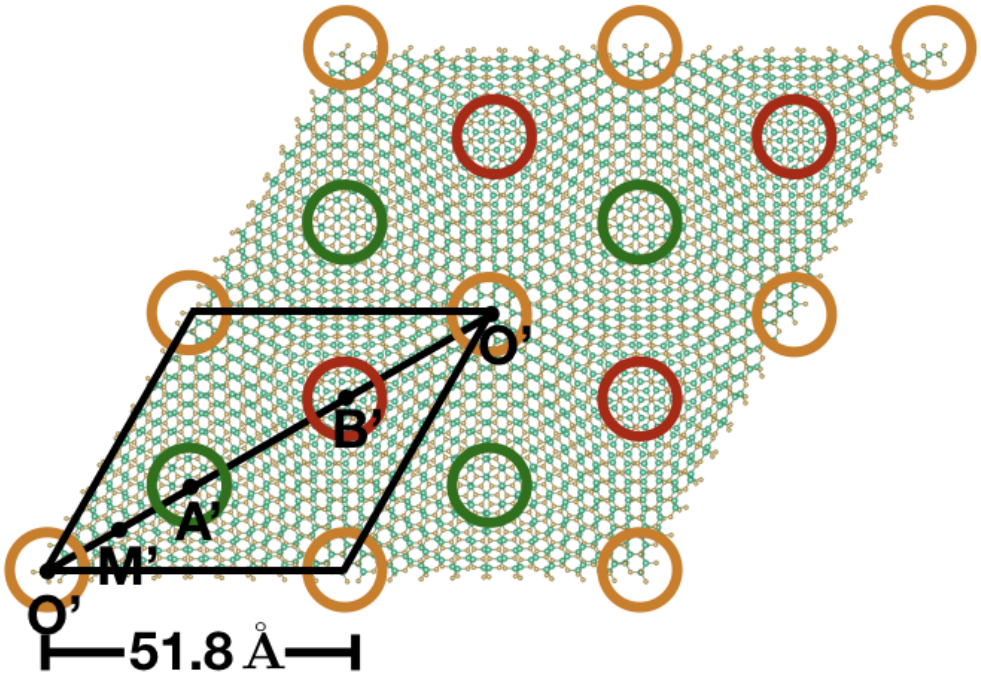

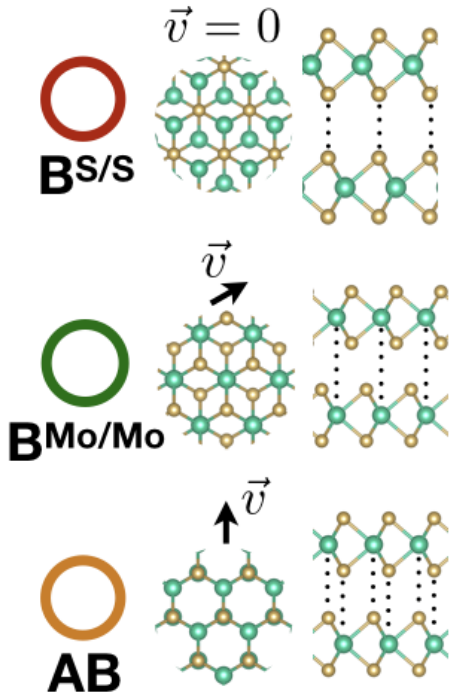

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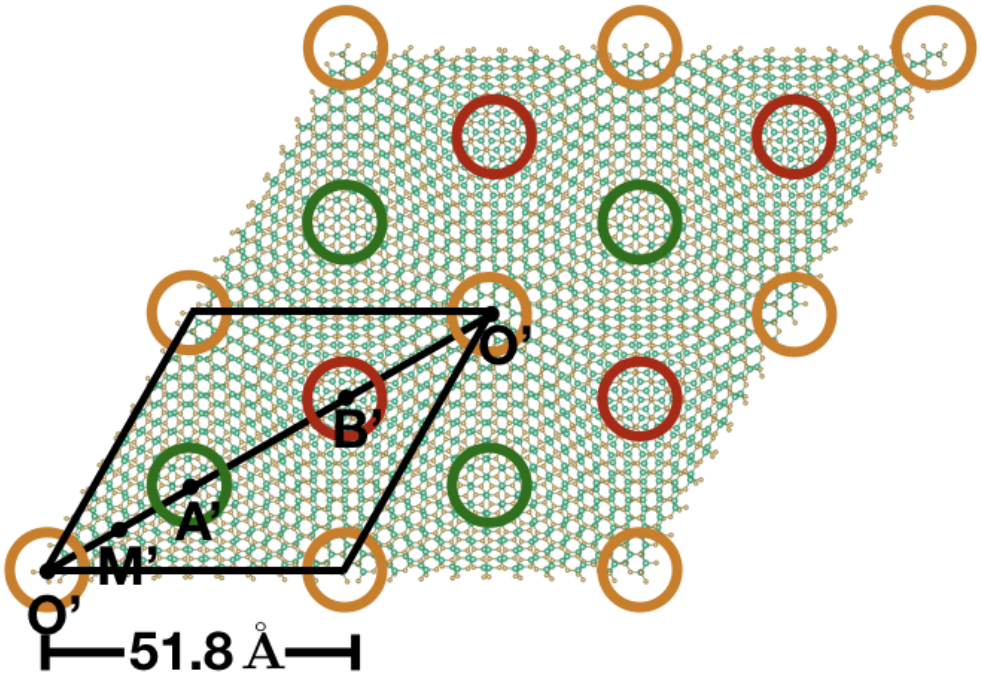
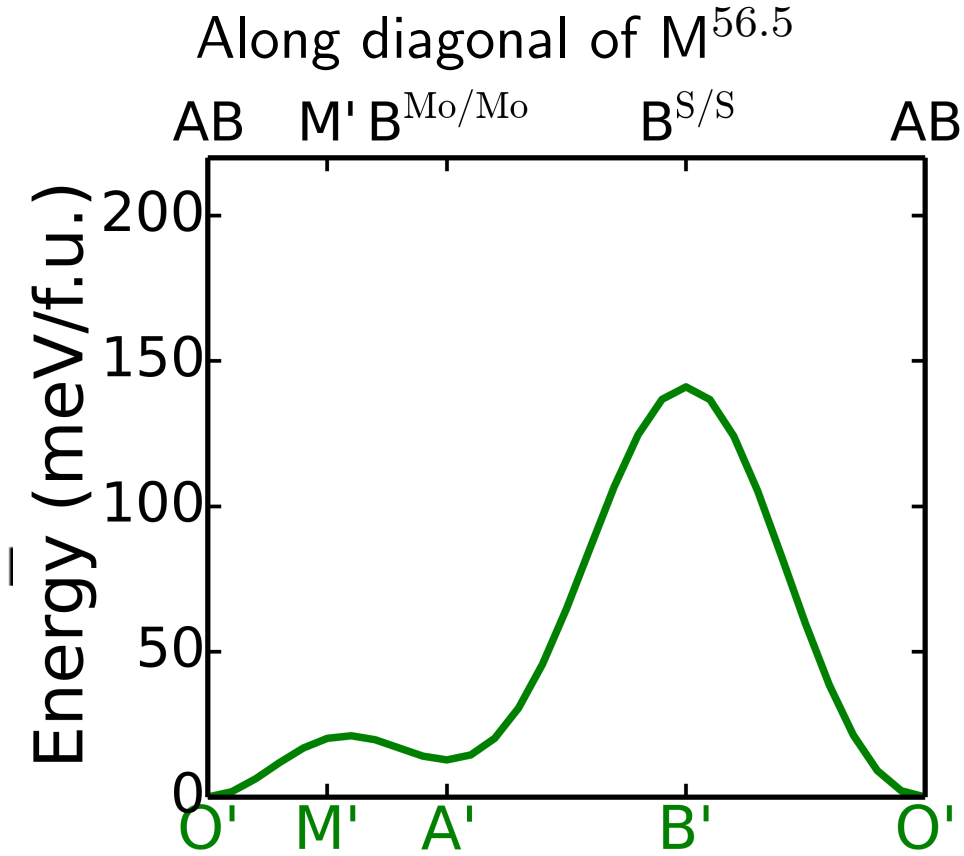
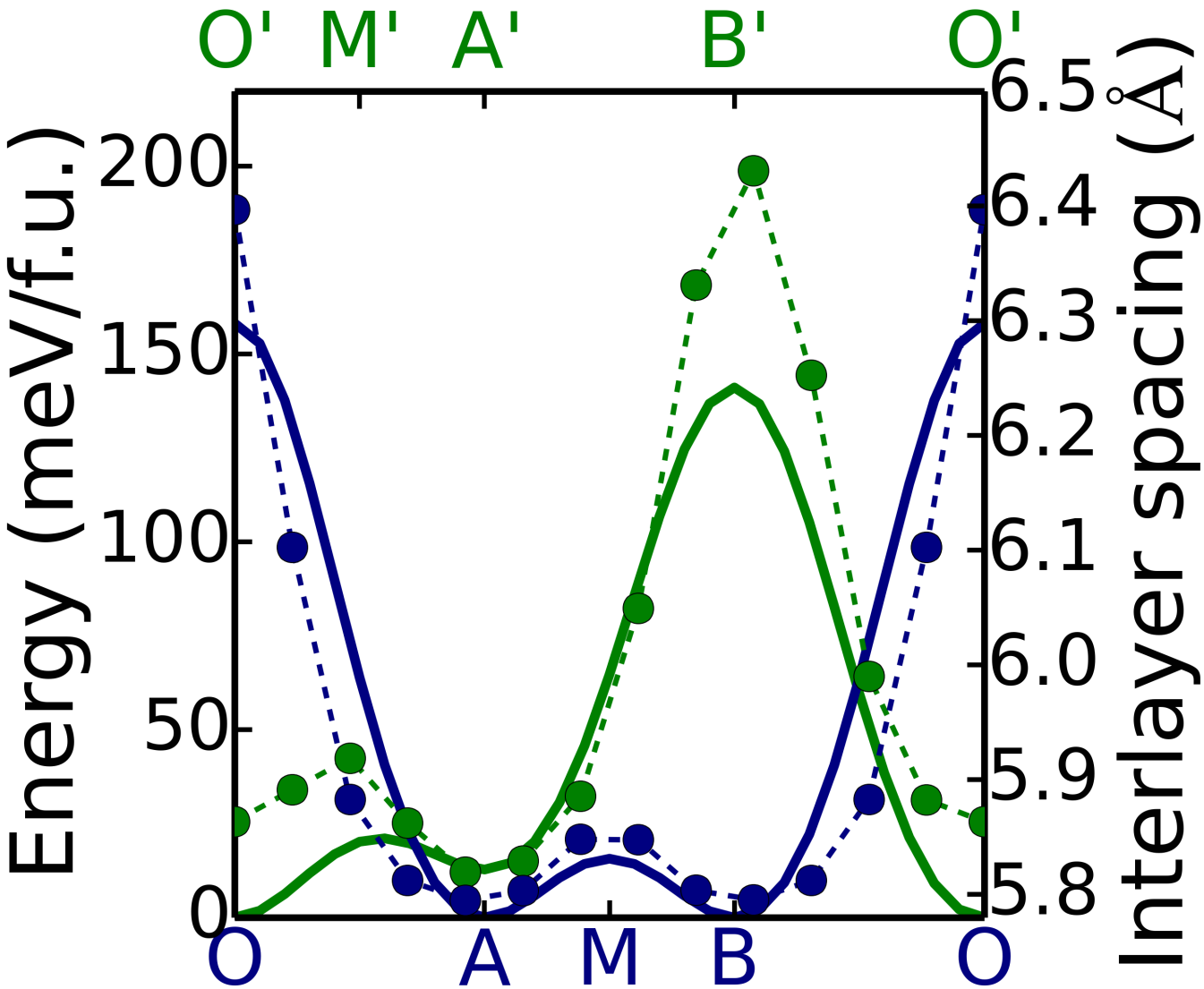
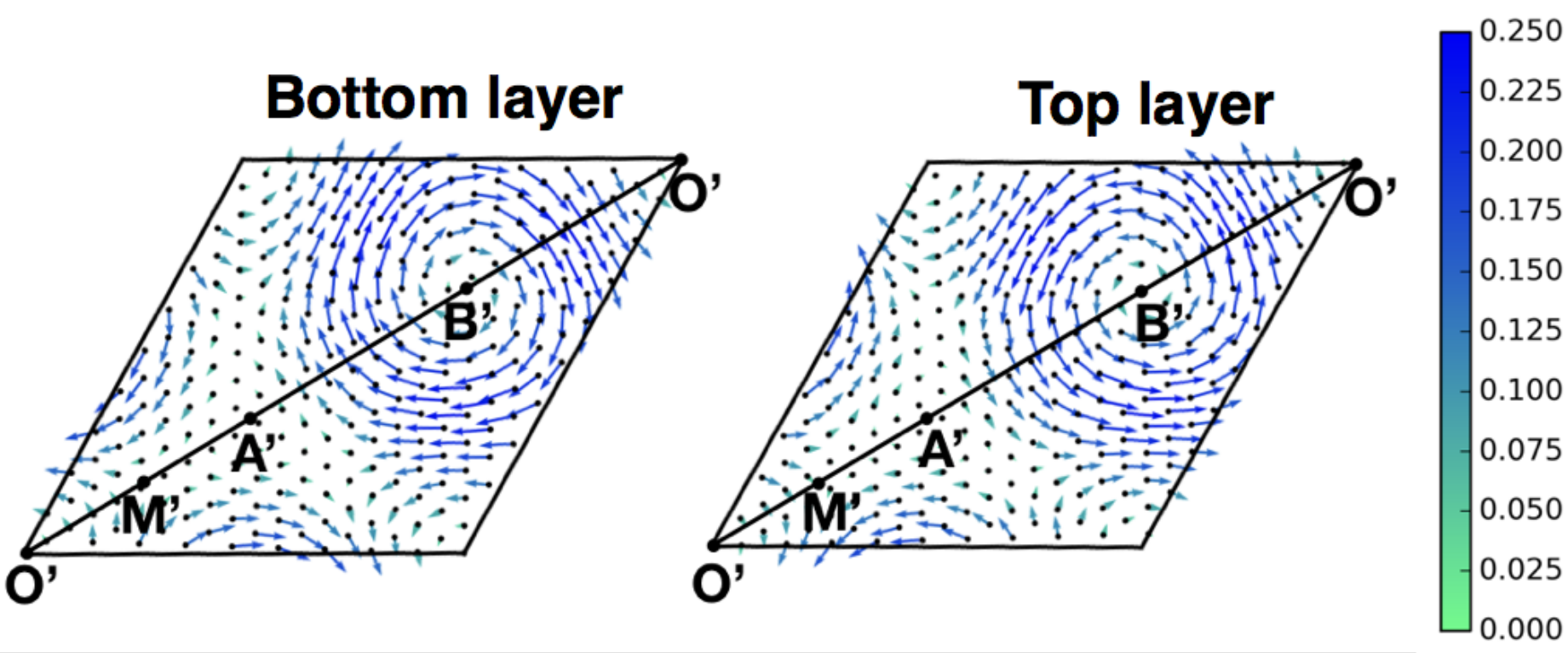




Interlayer spacings (ILS) in the Moiré



In-plane displacements, $M^{56.5}$



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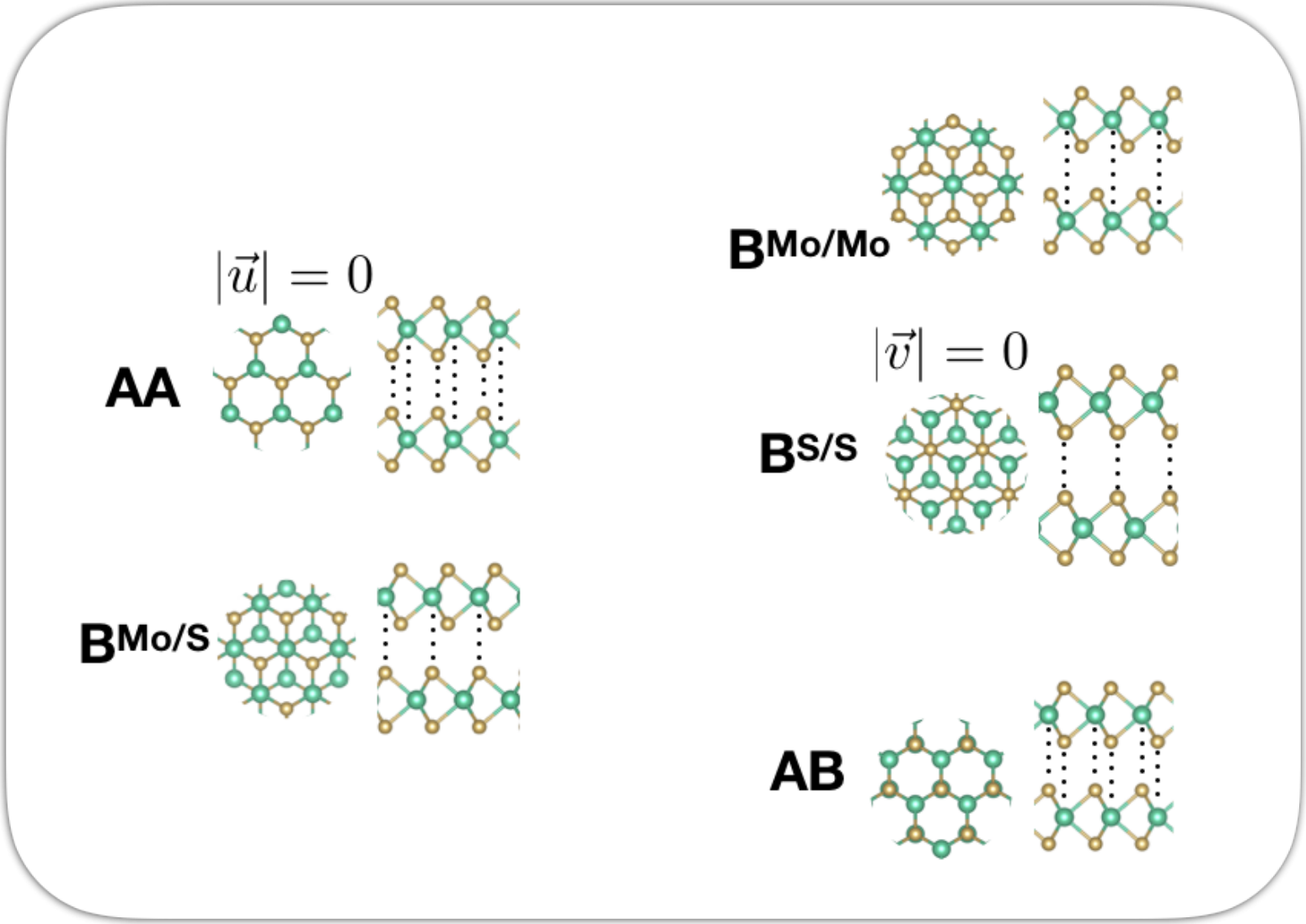
- $\vec{u}$ for angles close to 0°, and $\vec{v}$ for angles close to 60°

Order-parameter



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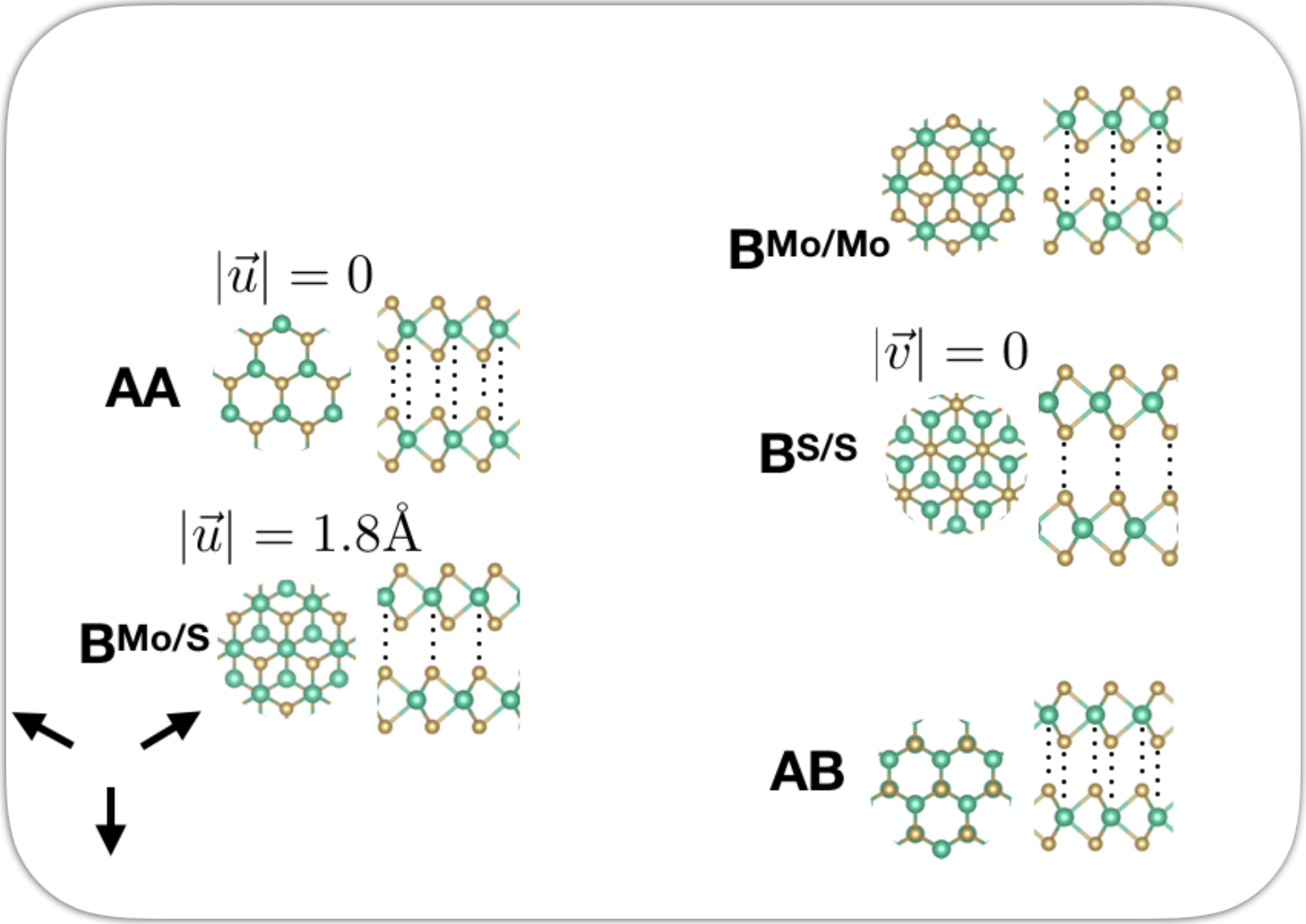

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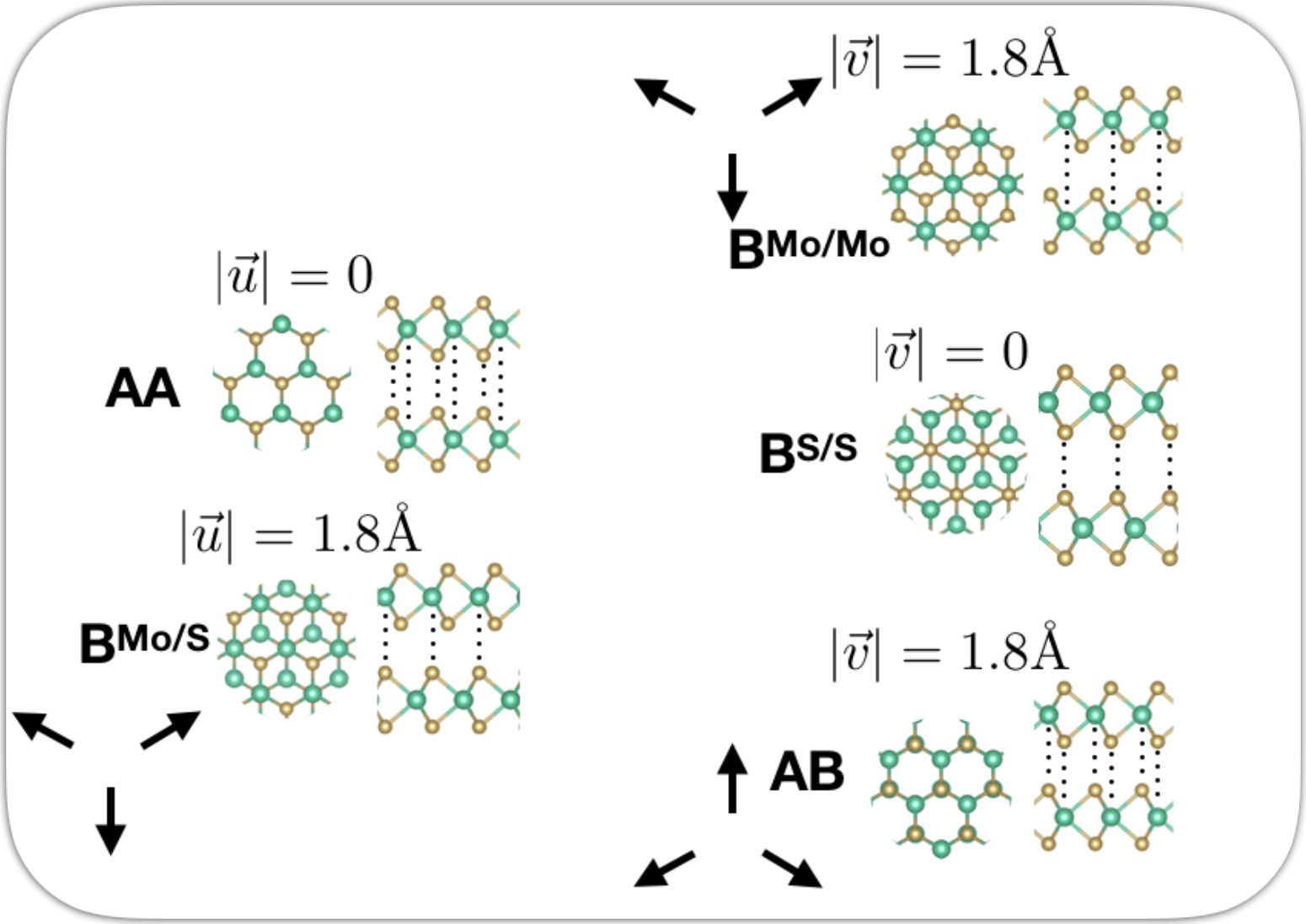
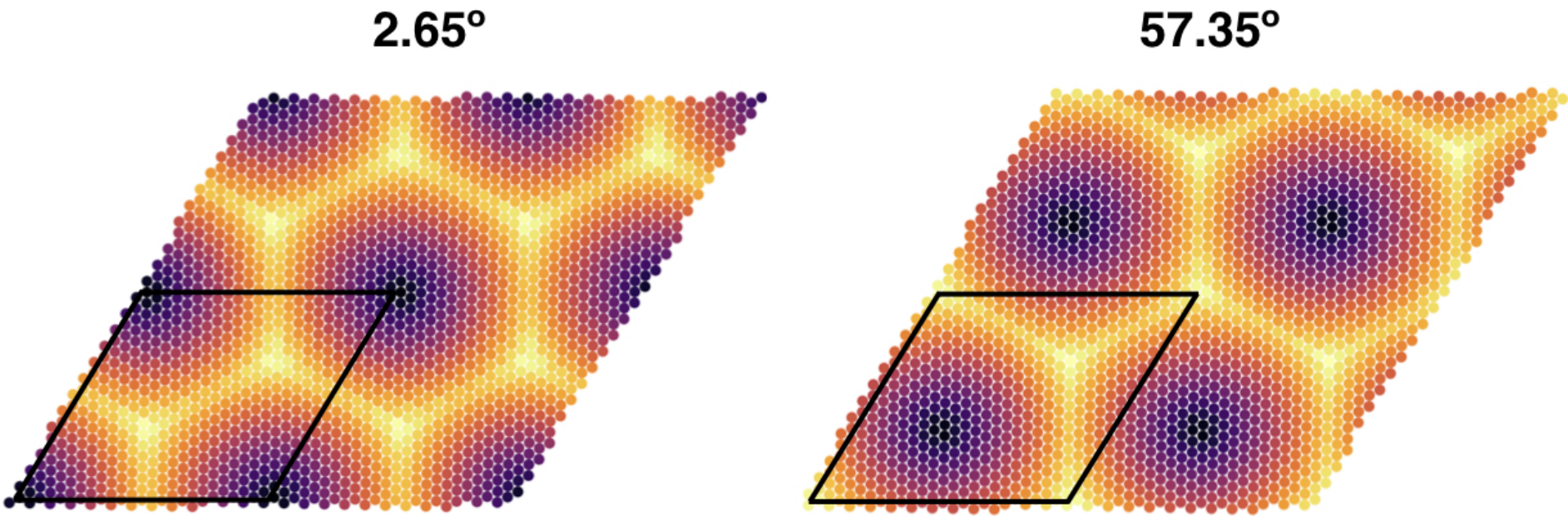


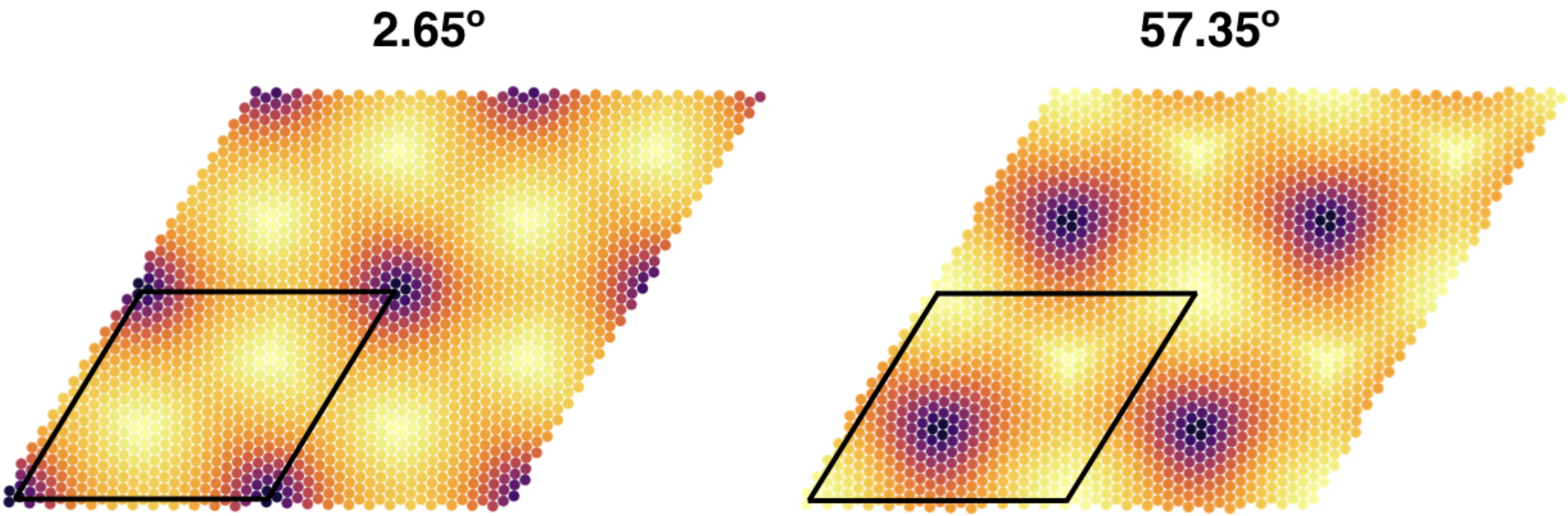
Order-parameter distribution

Unrelaxed:



Order-parameter distribution

Upon relaxation, trade-off between induced strain and energy minimization by displacing to a stable stacking.



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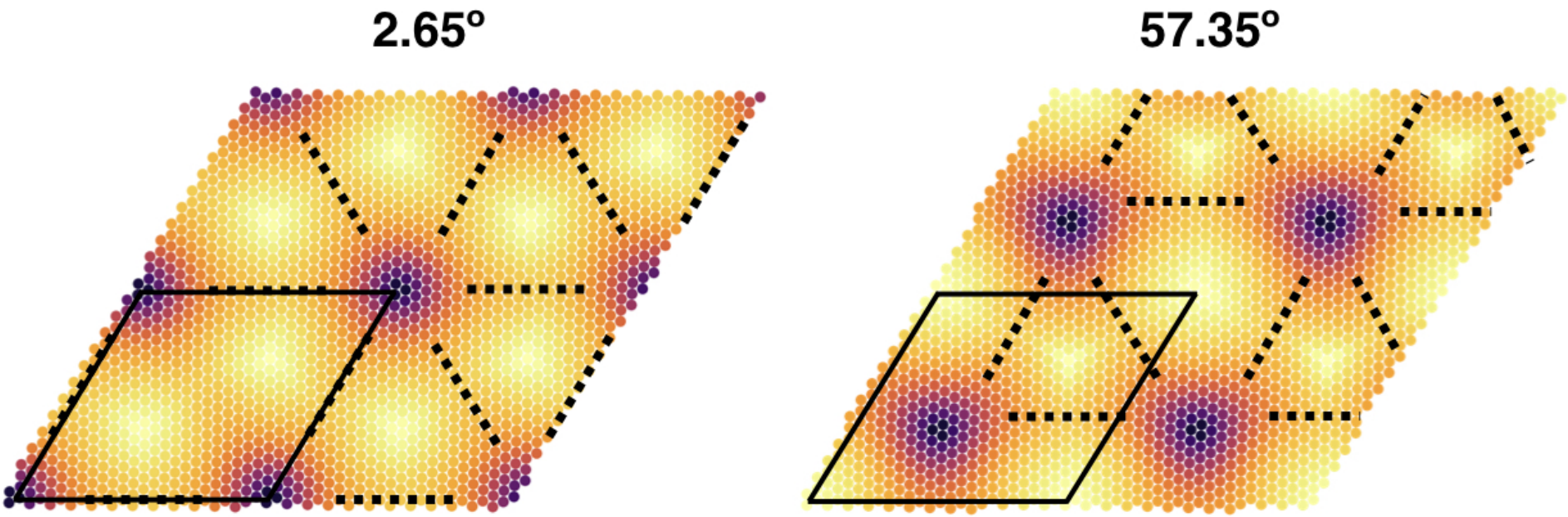
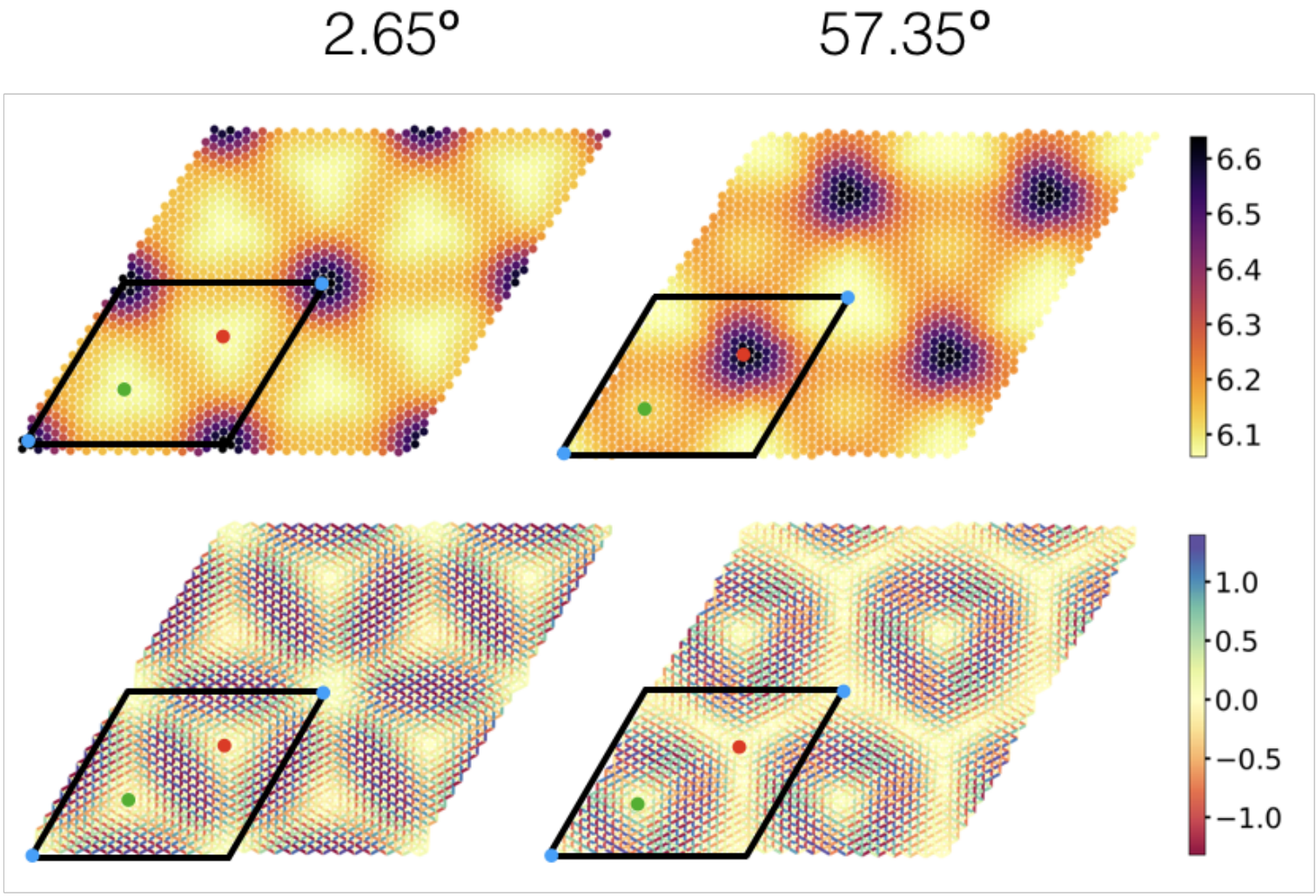
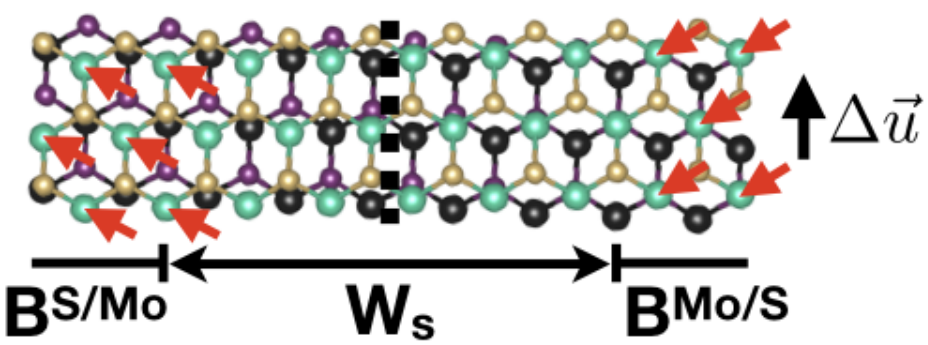
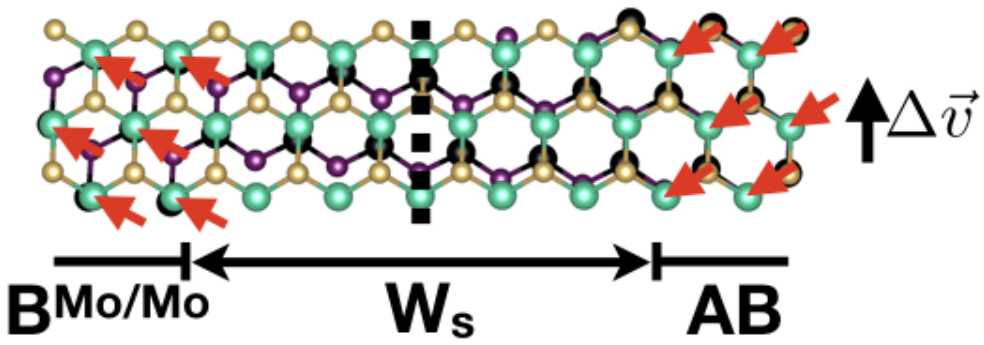


Interlayer spacing and strain distribution

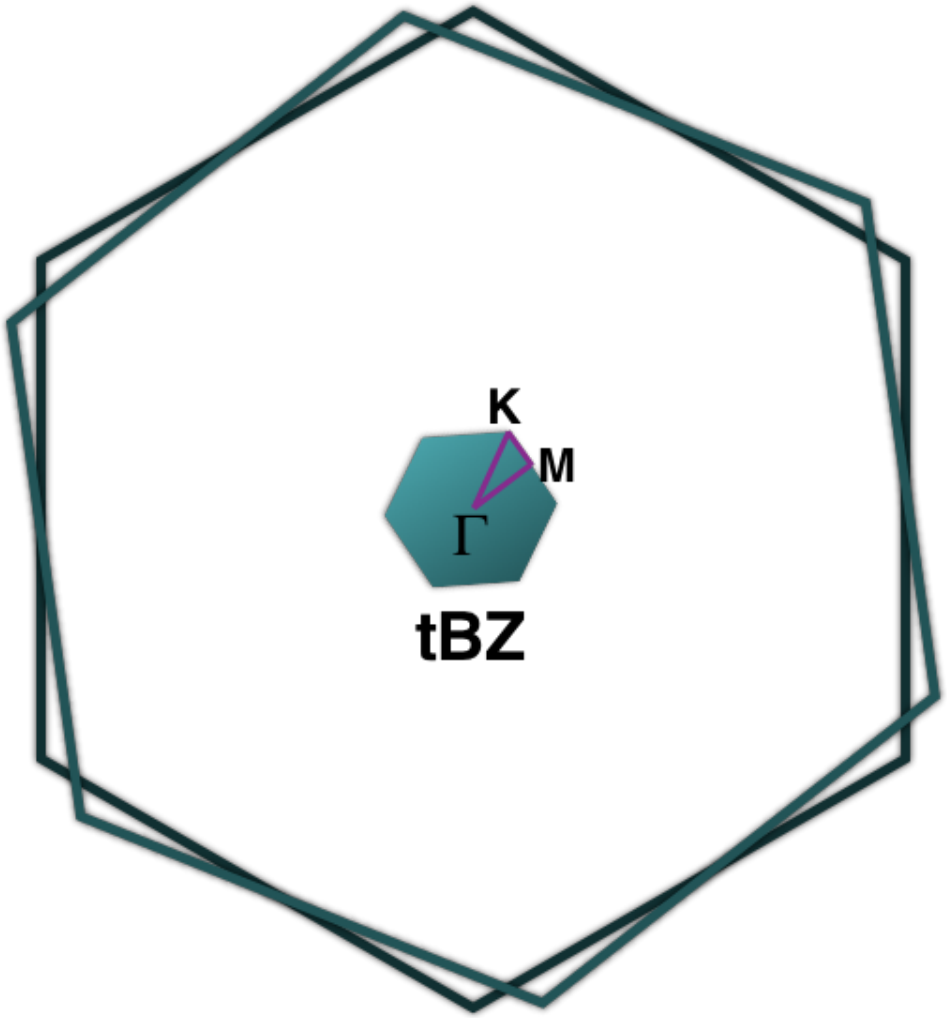


Shear-strain soliton

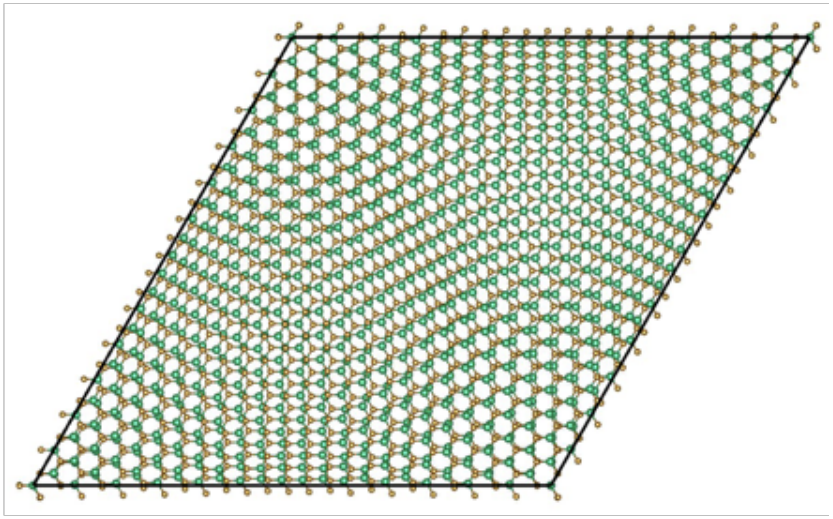




Electronic structure



Twist angle: 2.6°



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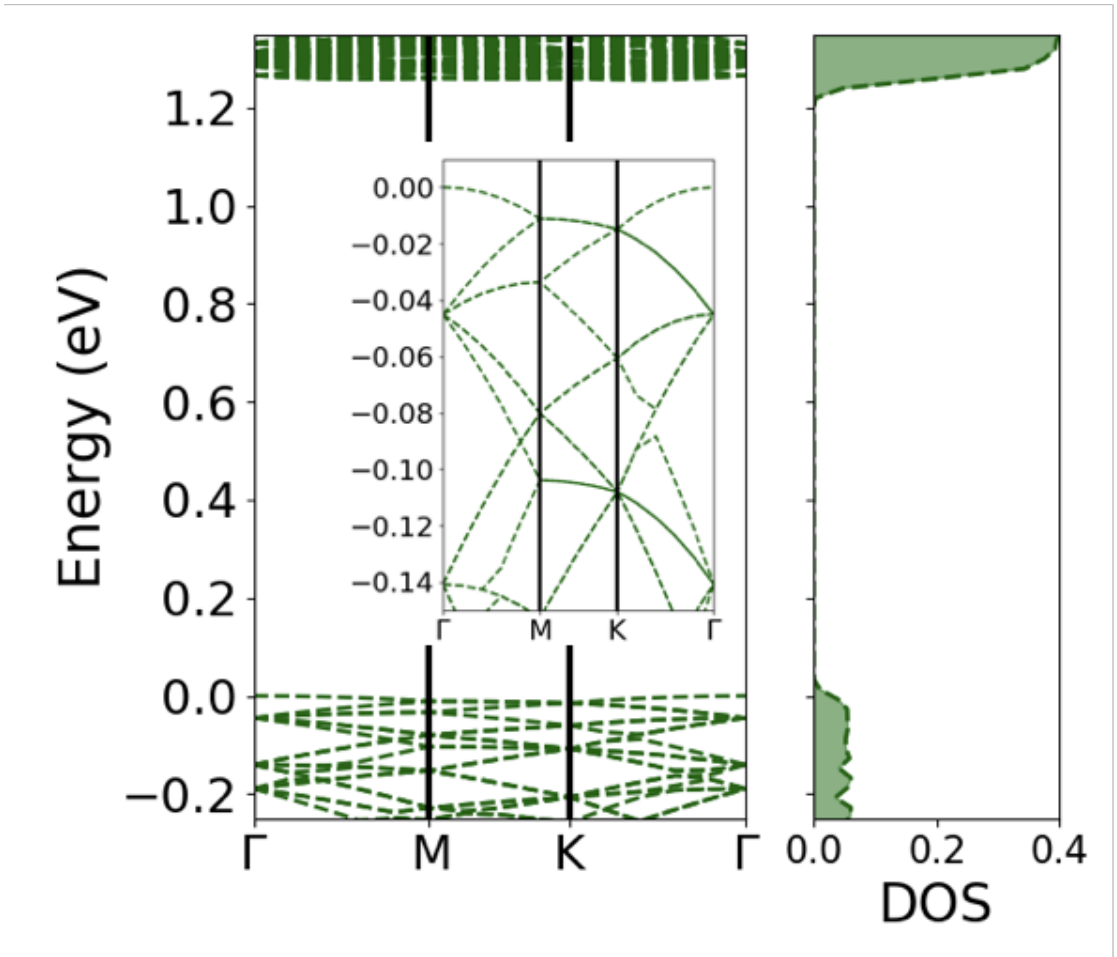
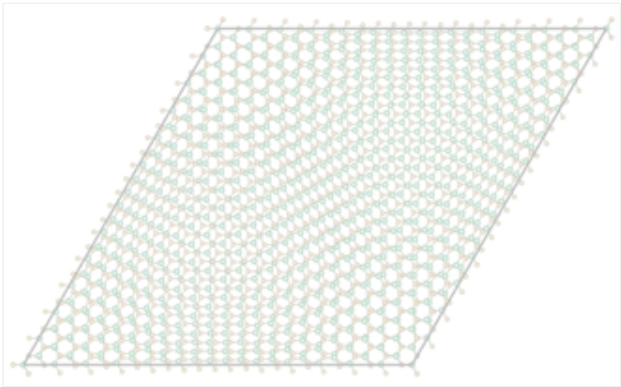
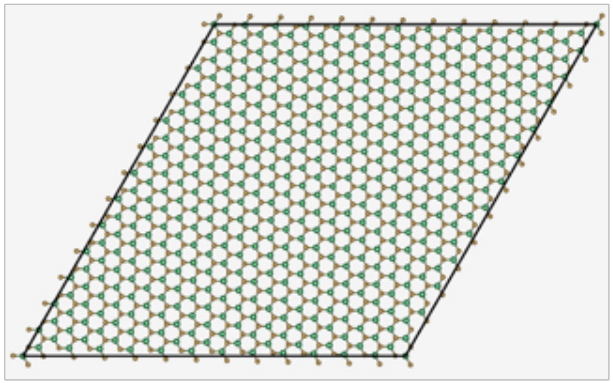


2.65° moiré superlattice



Pristine AB superlattice



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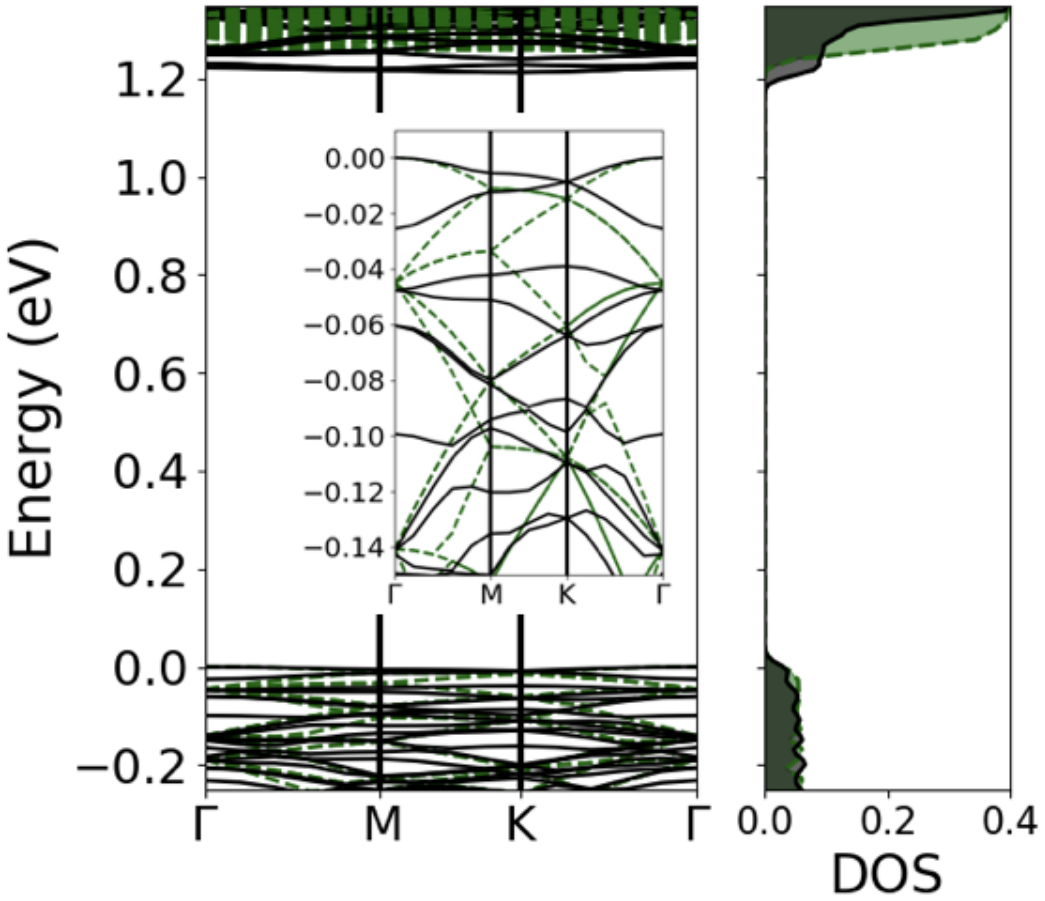

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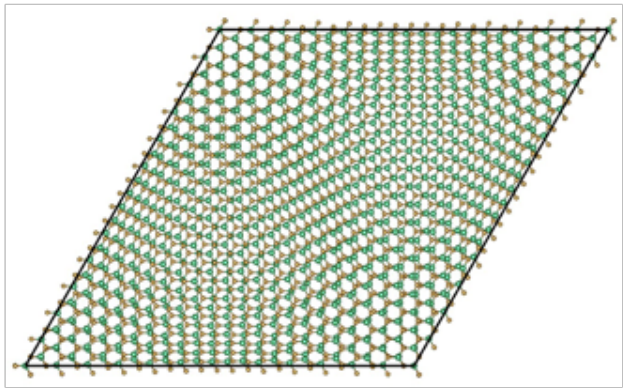

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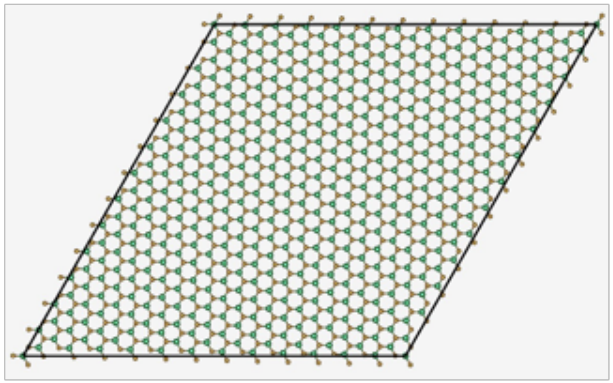
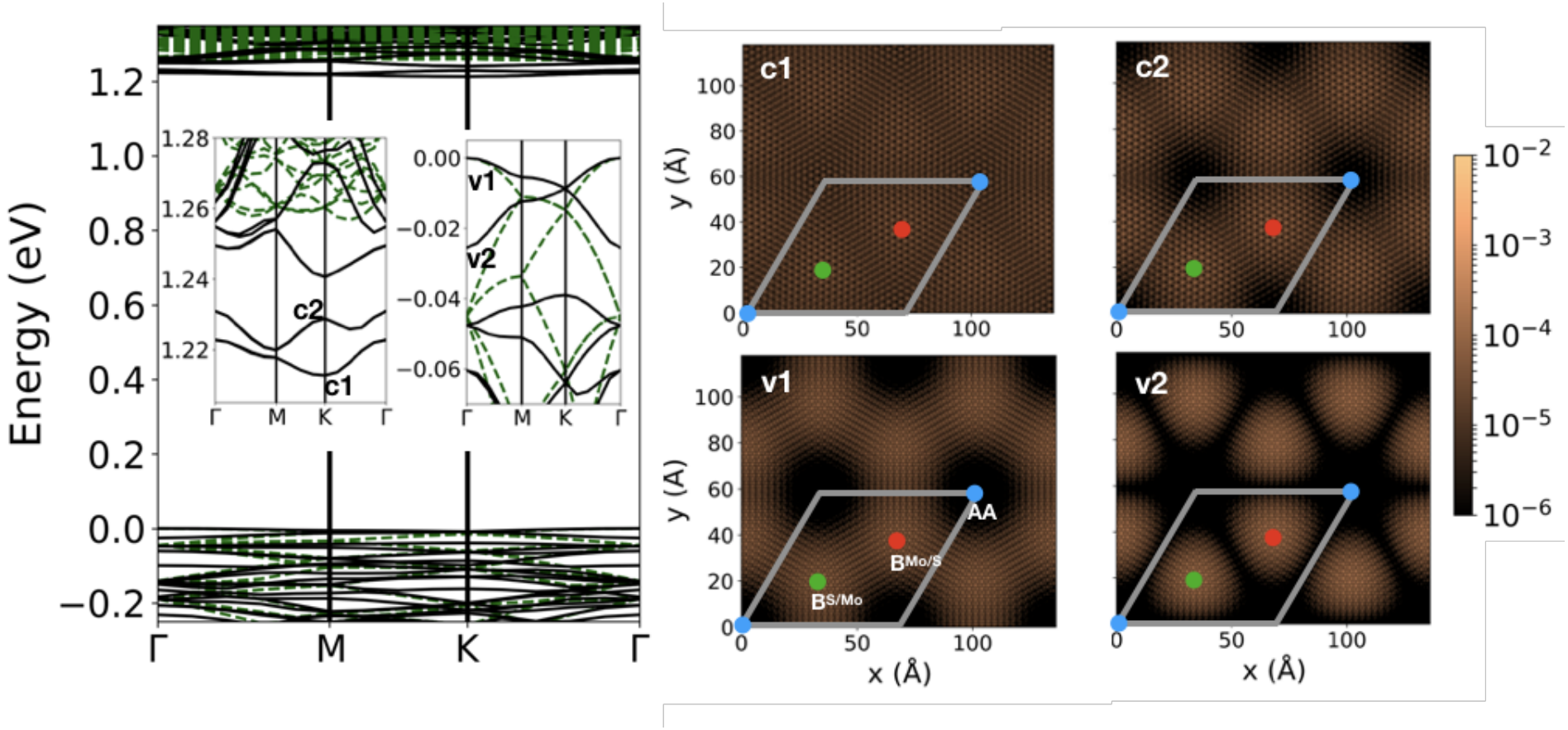
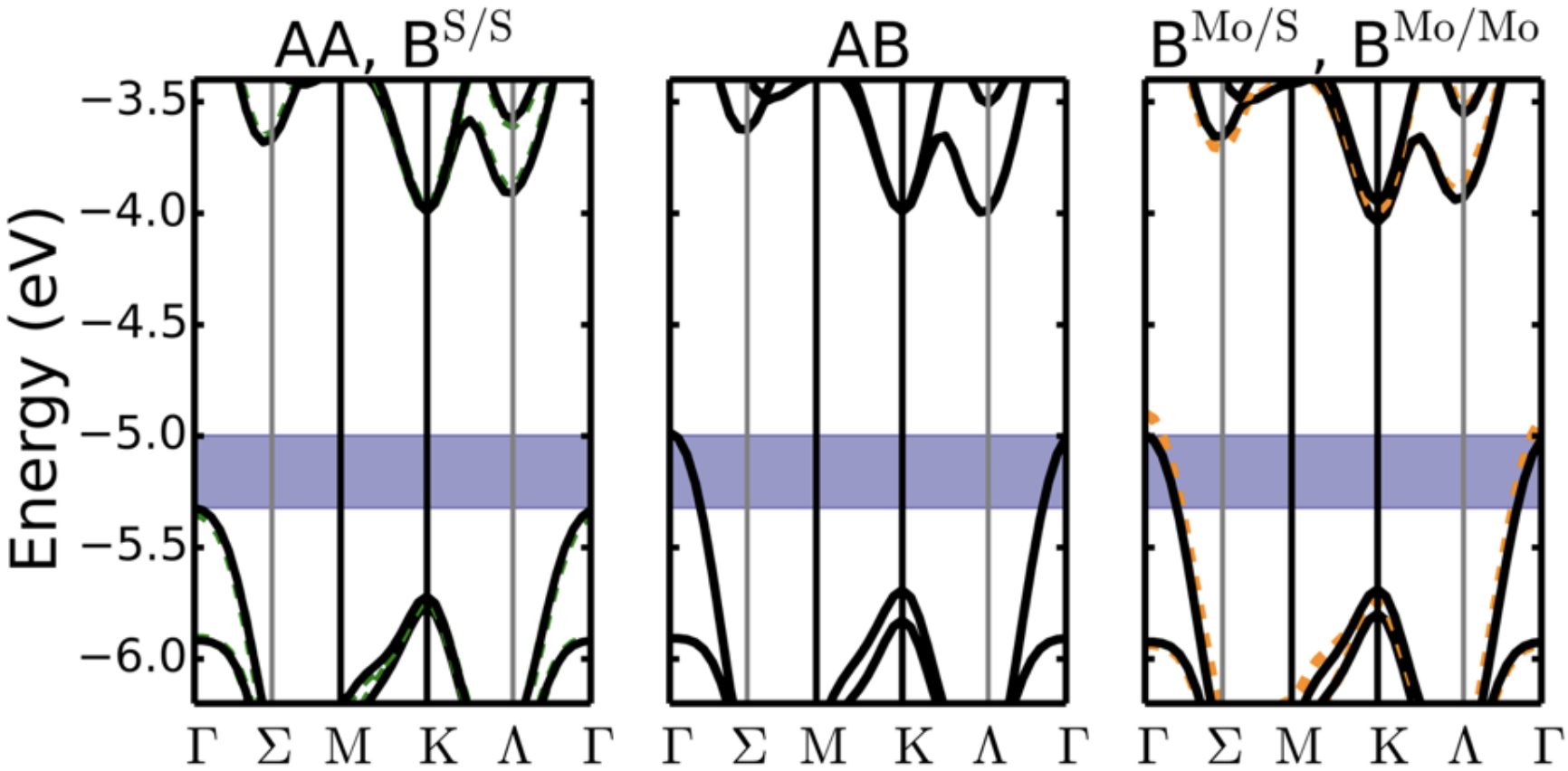


Localisation, 2.65° MSL



Electronic structure of individual stackings

At their equilibrium interlayer spacing.



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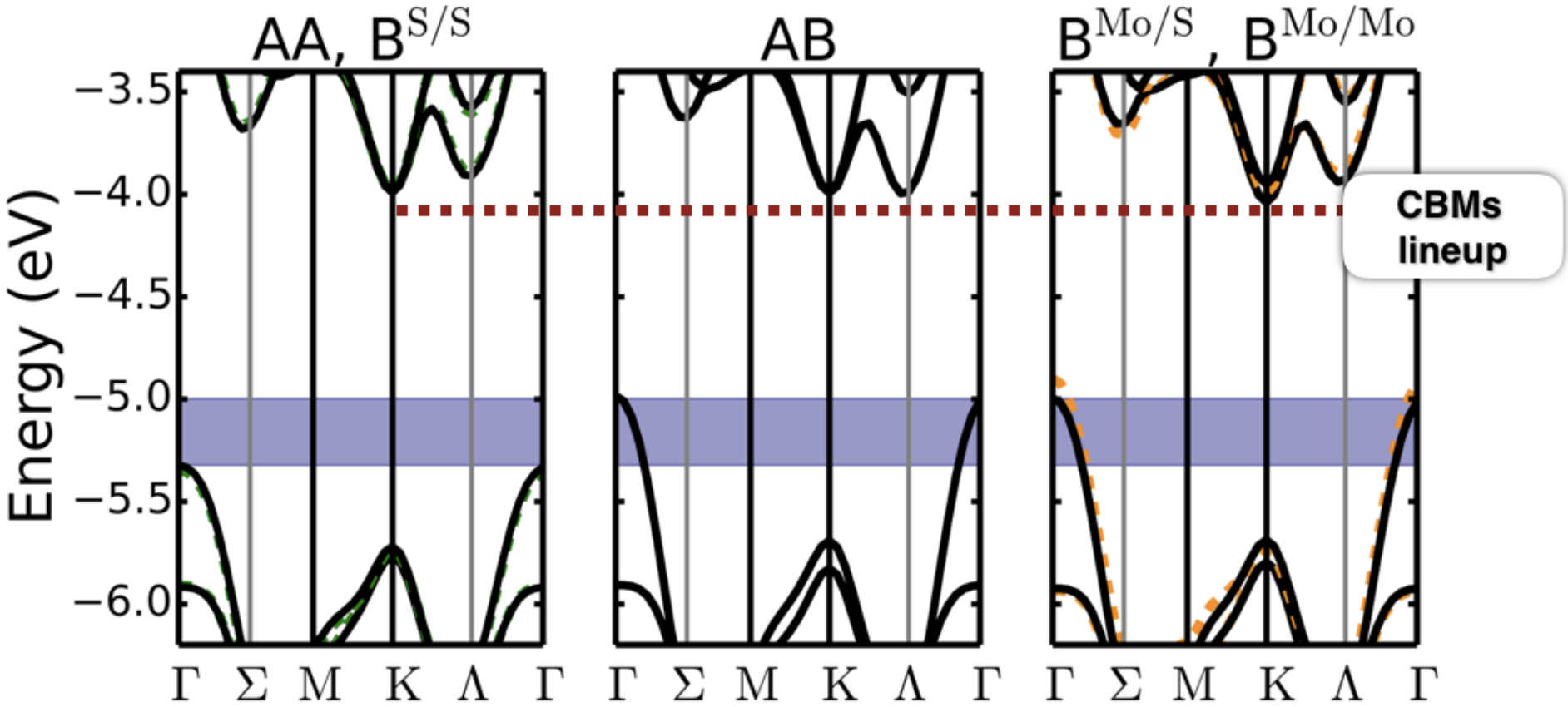

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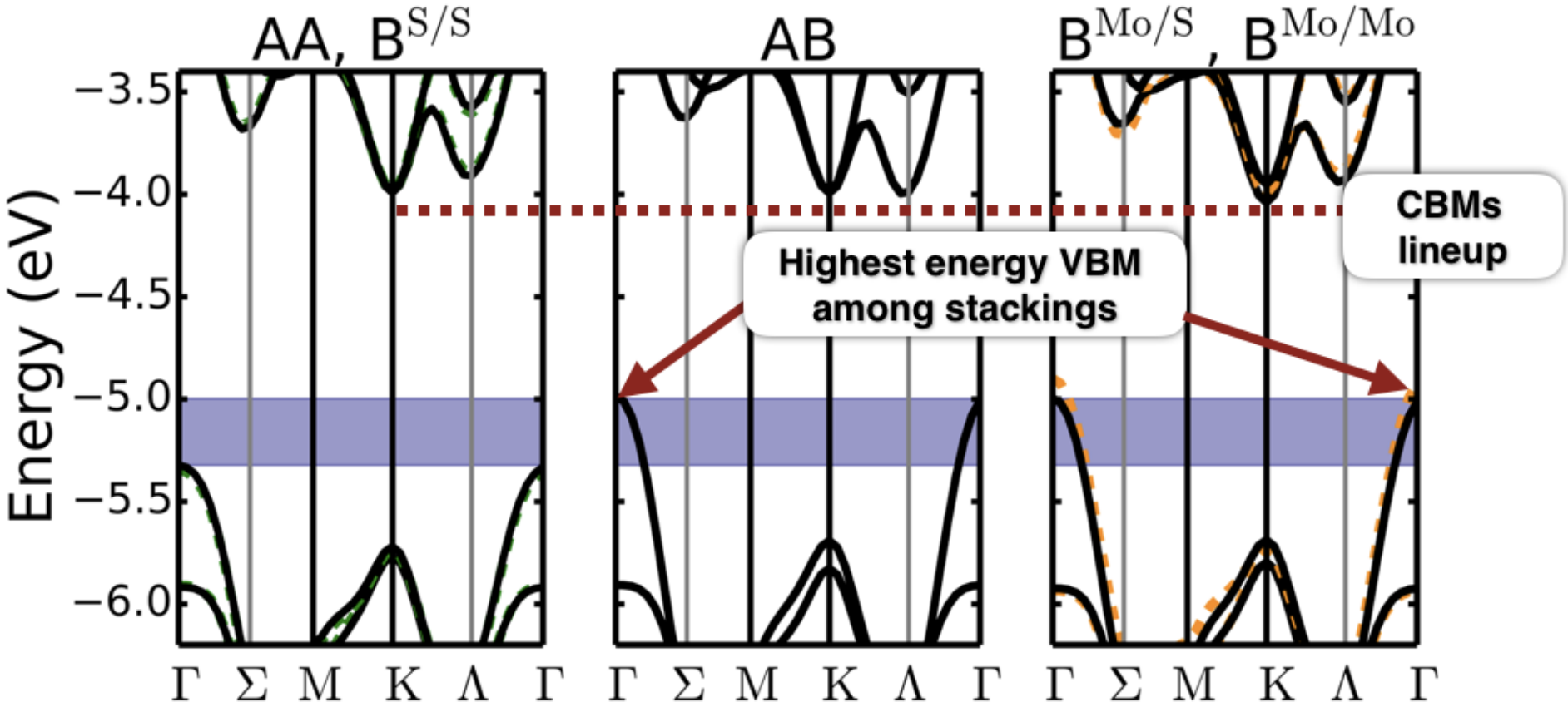
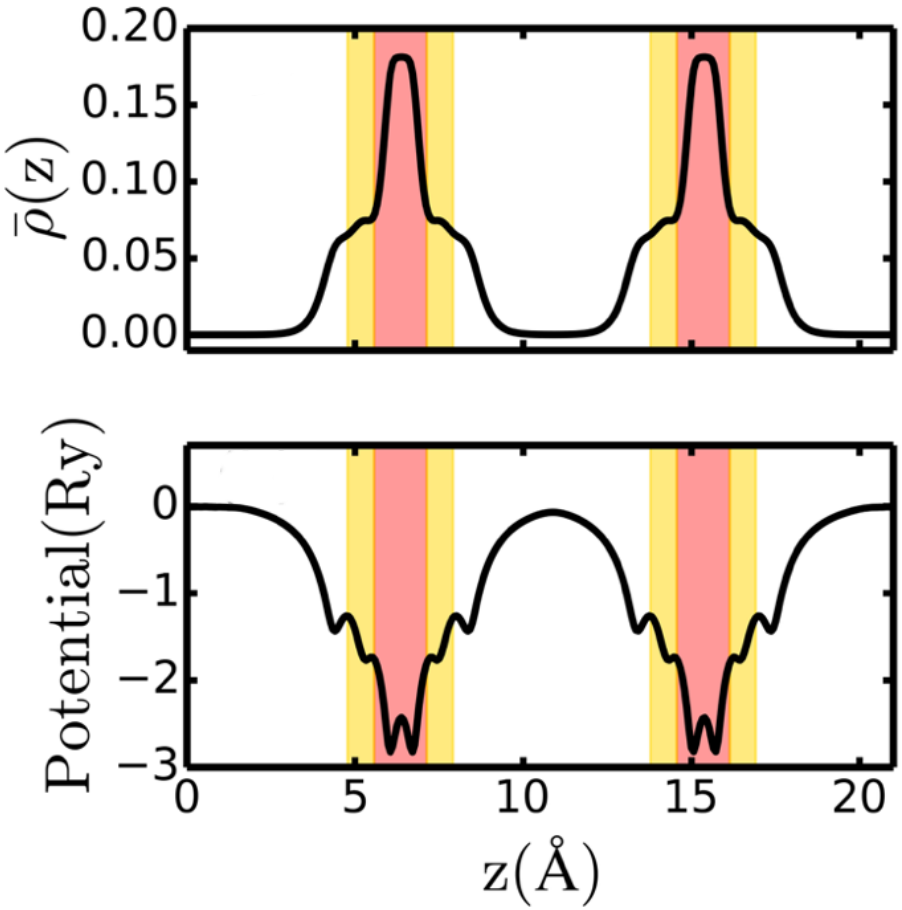
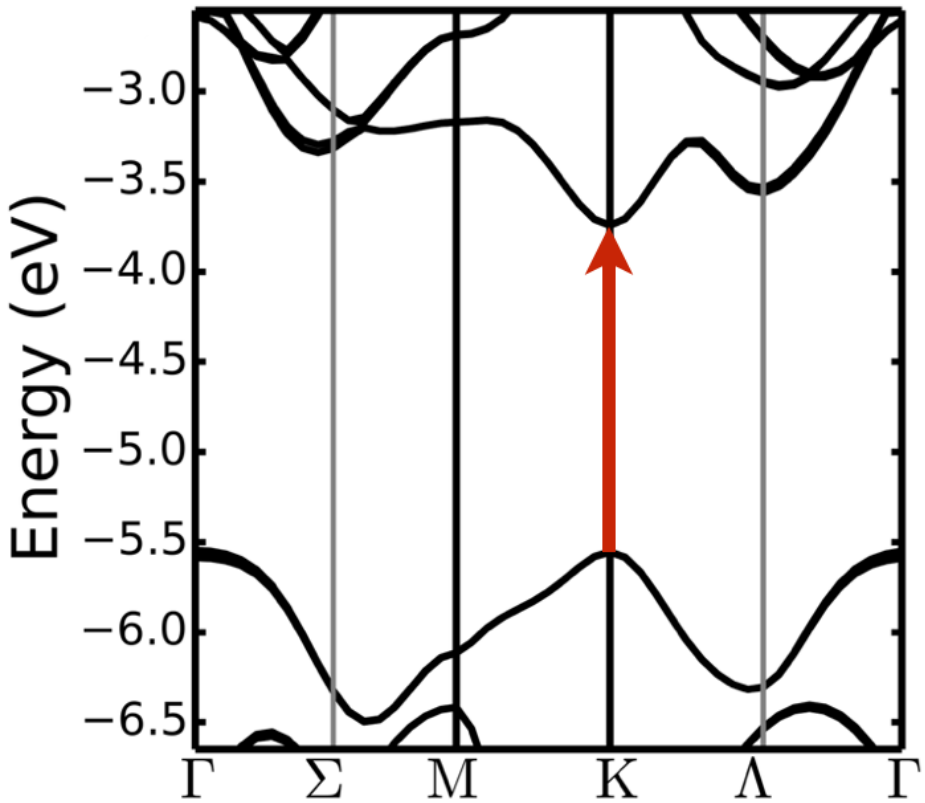


Hybridisation between layers

Barrier potential between layers: measure of the hybridisation between the layers.





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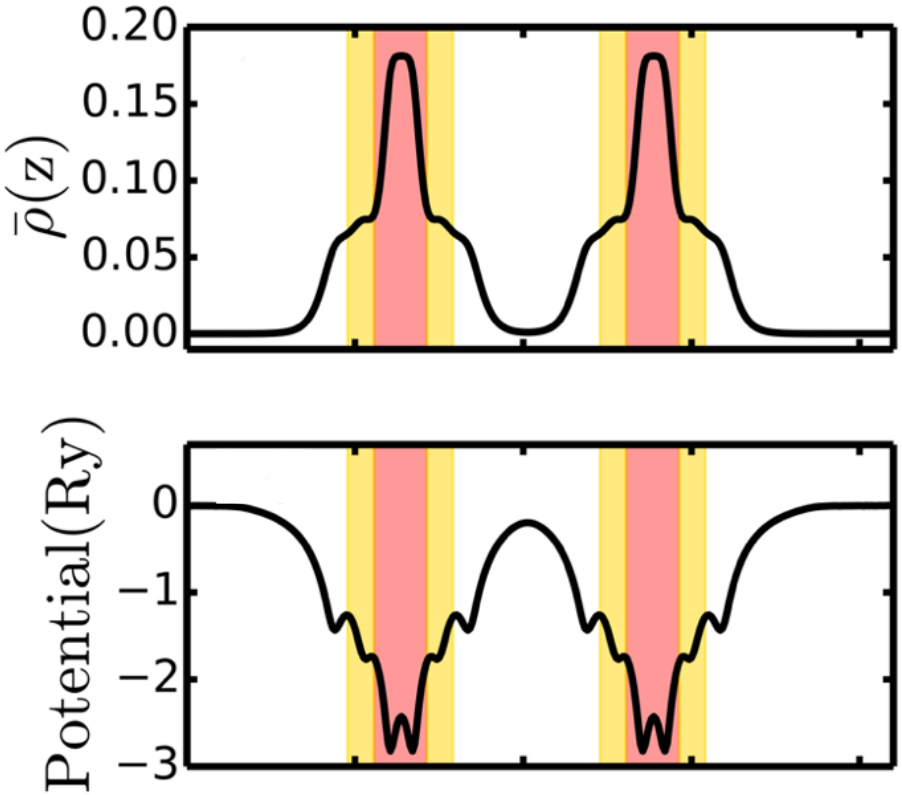

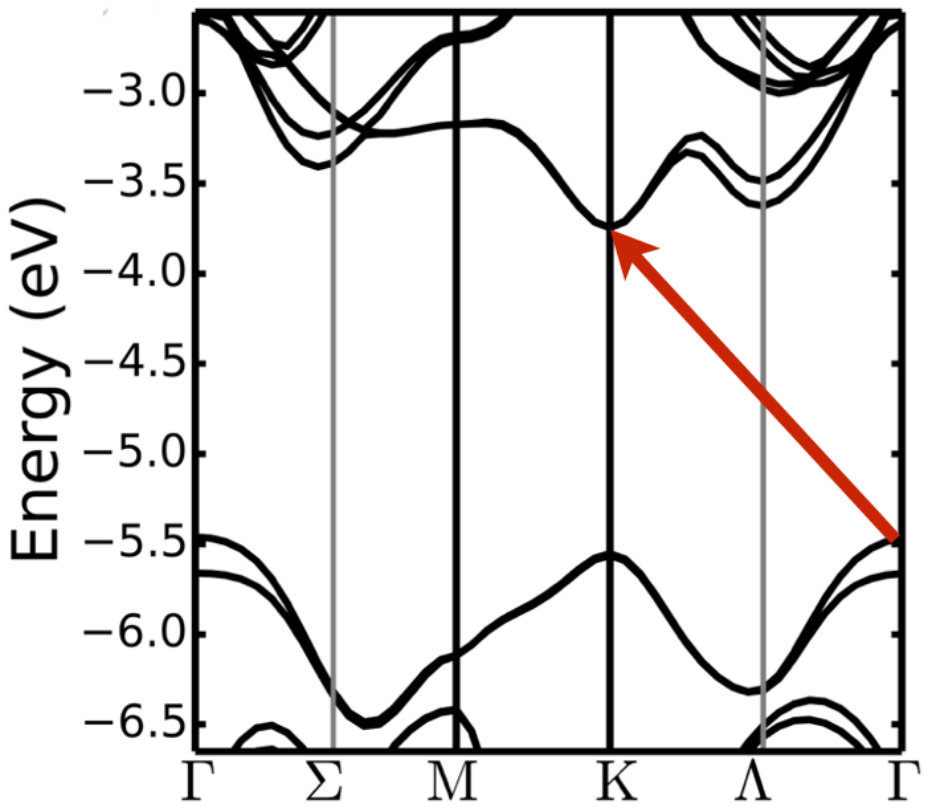

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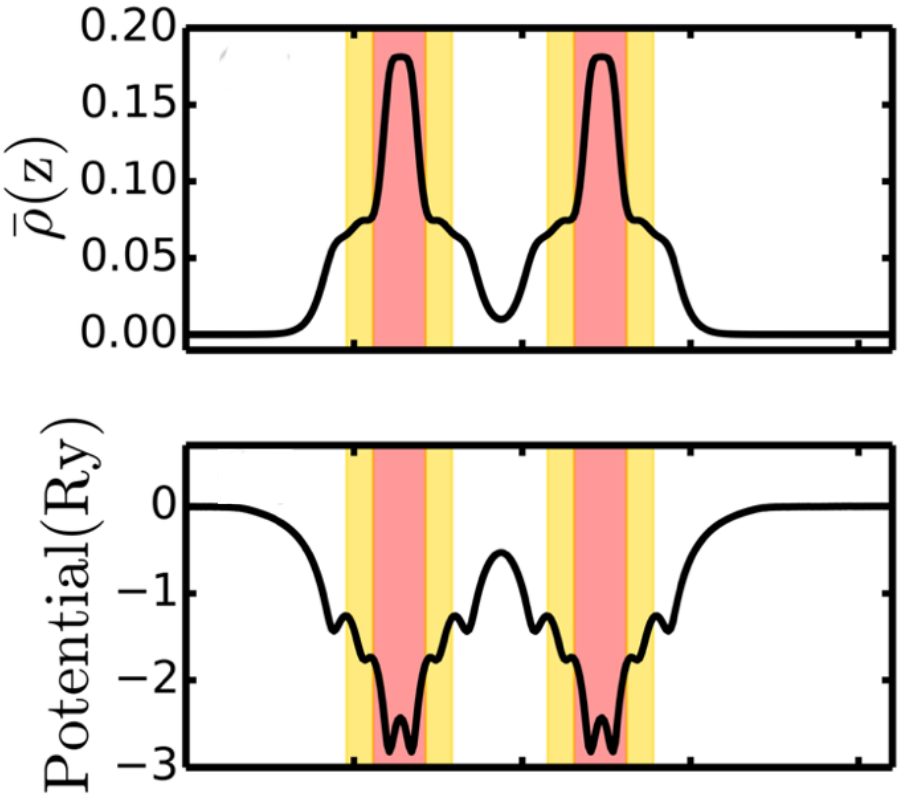
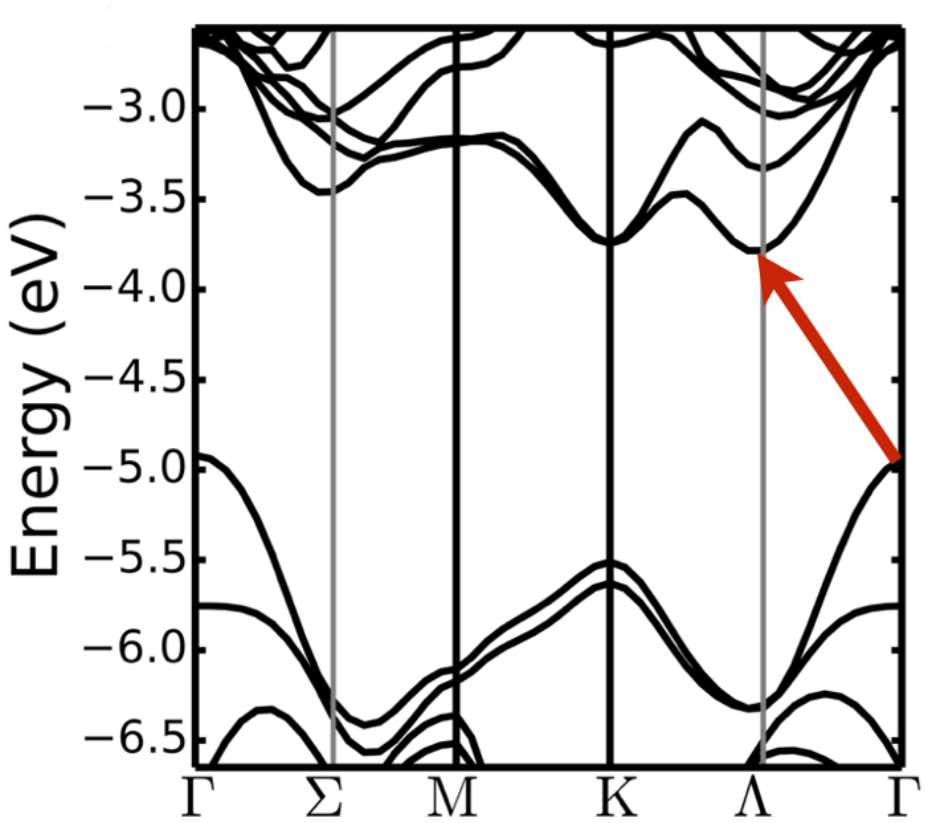
Barrier potential between layers: measure of the hybridisation between the layers.





Confining Potential

$$\Delta V(x,y) = V_{\mathrm{MSL}}(x,y) - \bar{V}_{\mathrm{AB}}$$

$$V_{\mathrm{MSL}}(x_0,y_0) = \int_{A_{uc}} \left(\frac{1}{2L_0} \int_{-L_0}^{L_0} V_{\mathrm{MSL}}(x,y,z)dz \right) dxdy$$

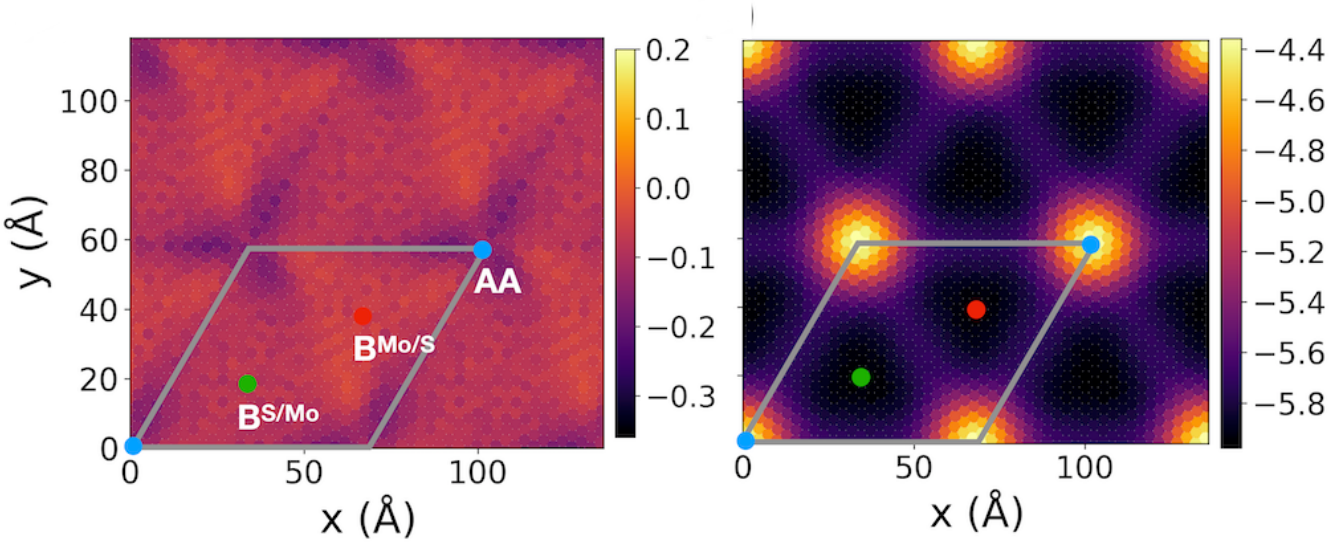
is the z and macroscopic averaged potential in the MSL.

$\bar{V}_{\mathrm{AB}}$ is unit-cell averaged potential of AB stacking.

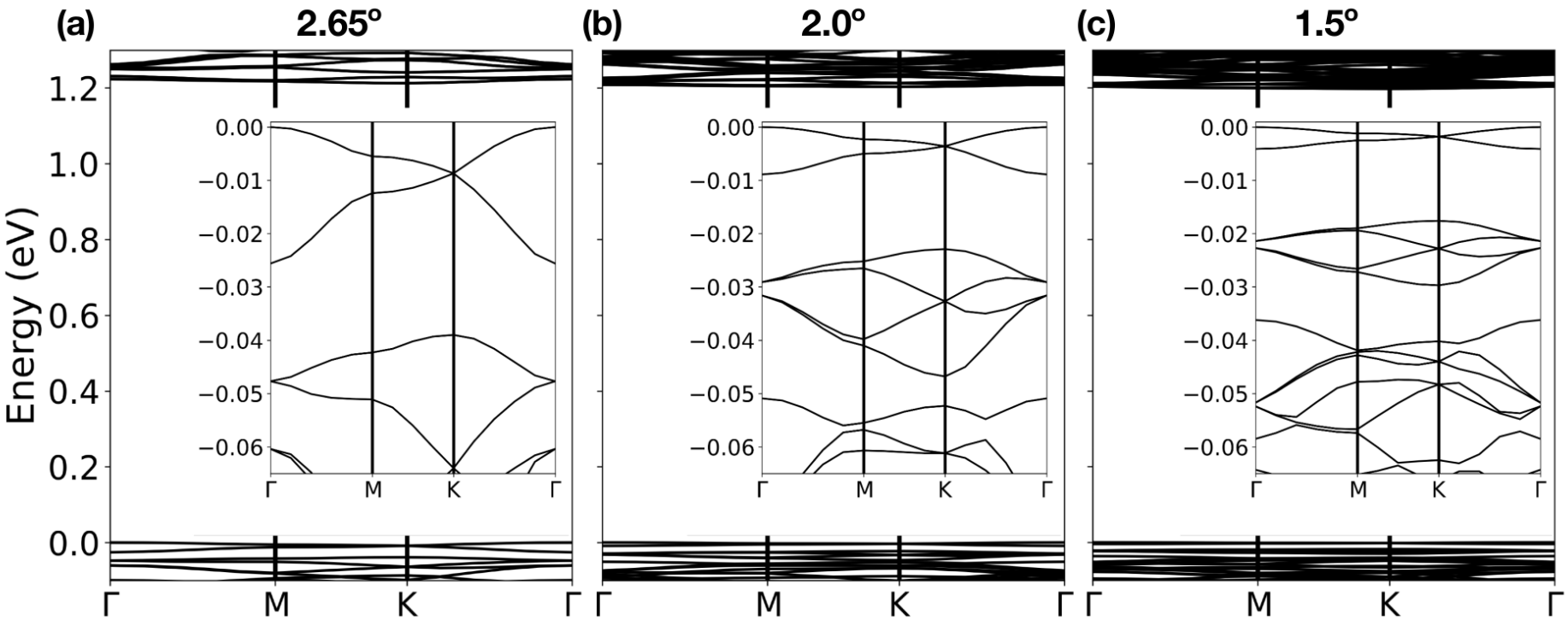
Inhomogeneous hybridisation in moiré

Localization governed by local barrier potential between the layers:

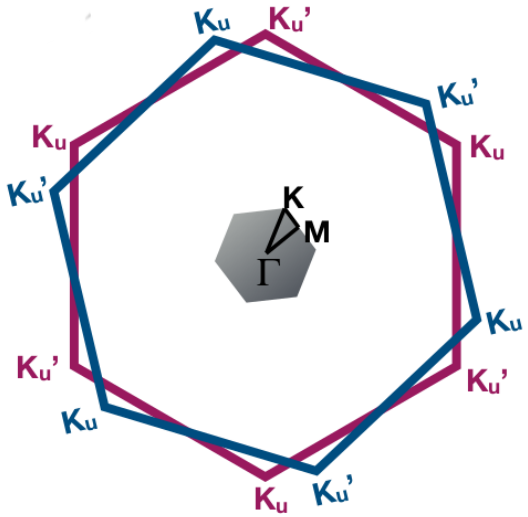
Confining potential Inhomogeneous hybridization

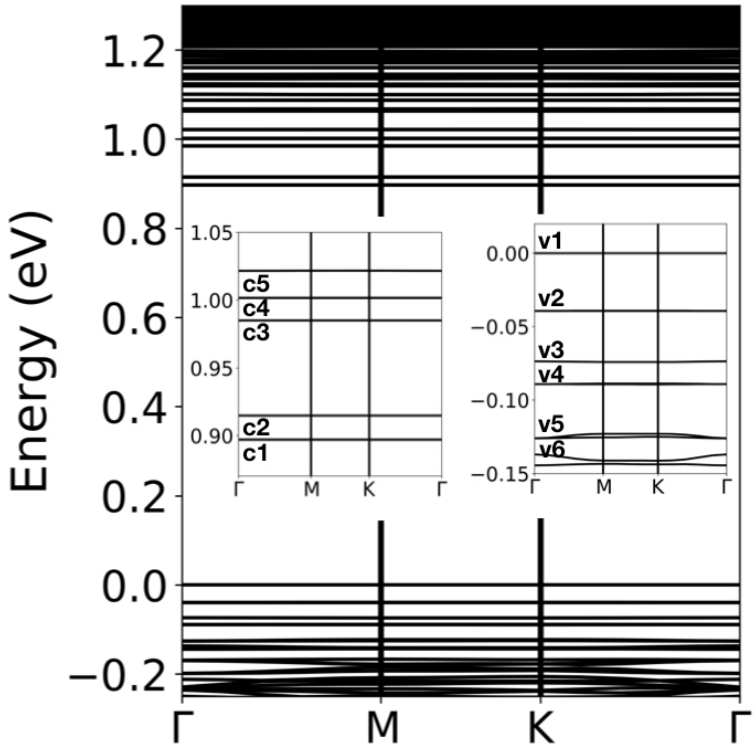


Evolution of band structure near 0°



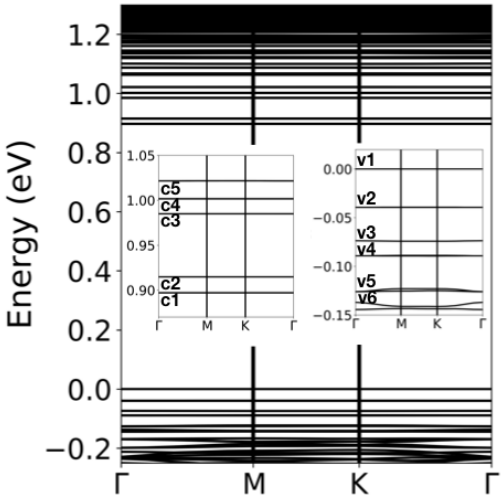
58° MSL


Ku
Ku'
Ku'
Ku
Ku'
Ku
Ku'
Ku
Ku
Ku'
K
M
Γ


Energy (eV)
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
Γ
M
K
Γ
1.05
1.00
0.95
0.90
c5
c4
c3
c2
c1
0.00
−0.05
−0.10
−0.15
v1
v2
v3
v4
v5
v6

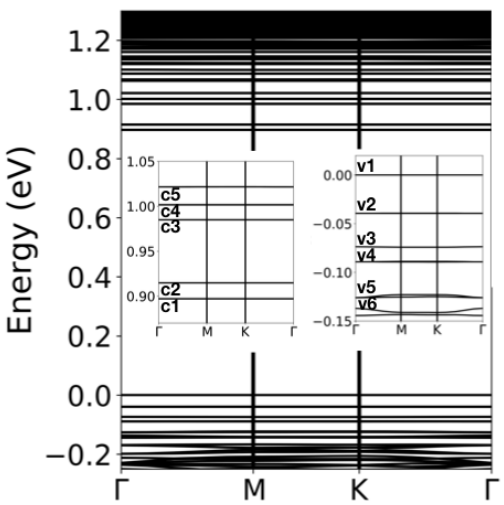
58° MSL

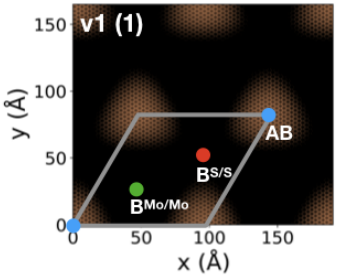
Equilateral triangle quantum well states.

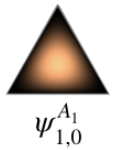


58° MSL

Equilateral triangle quantum well states.

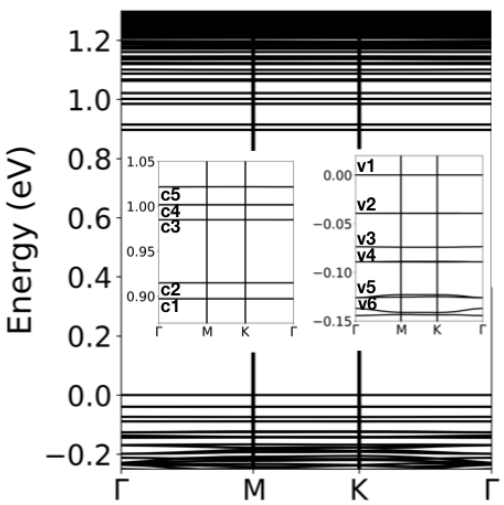


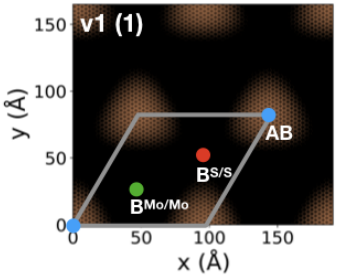




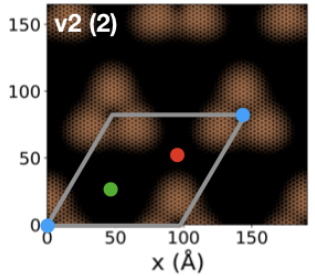
58° MSL

Equilateral triangle quantum well states.





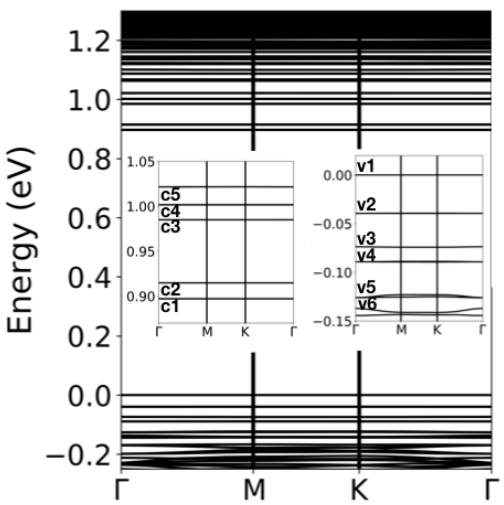
$\psi^{A_1}_{1,0}$

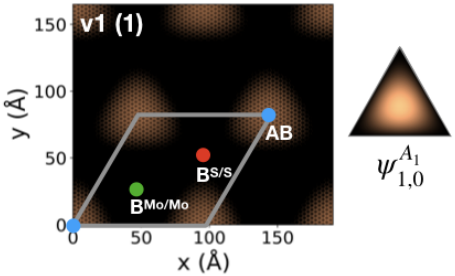


$\psi^{E}_{\frac{4}{3},\frac{1}{3}}$

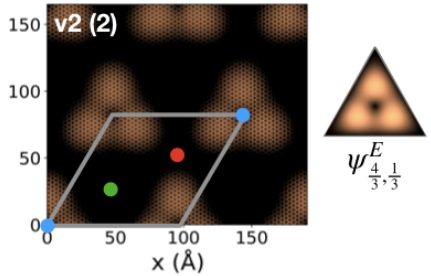
58° MSL

Equilateral triangle quantum well states.

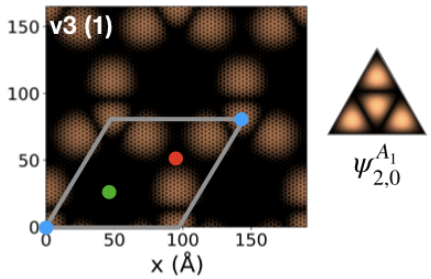




$\psi^{A_1}_{1,0}$



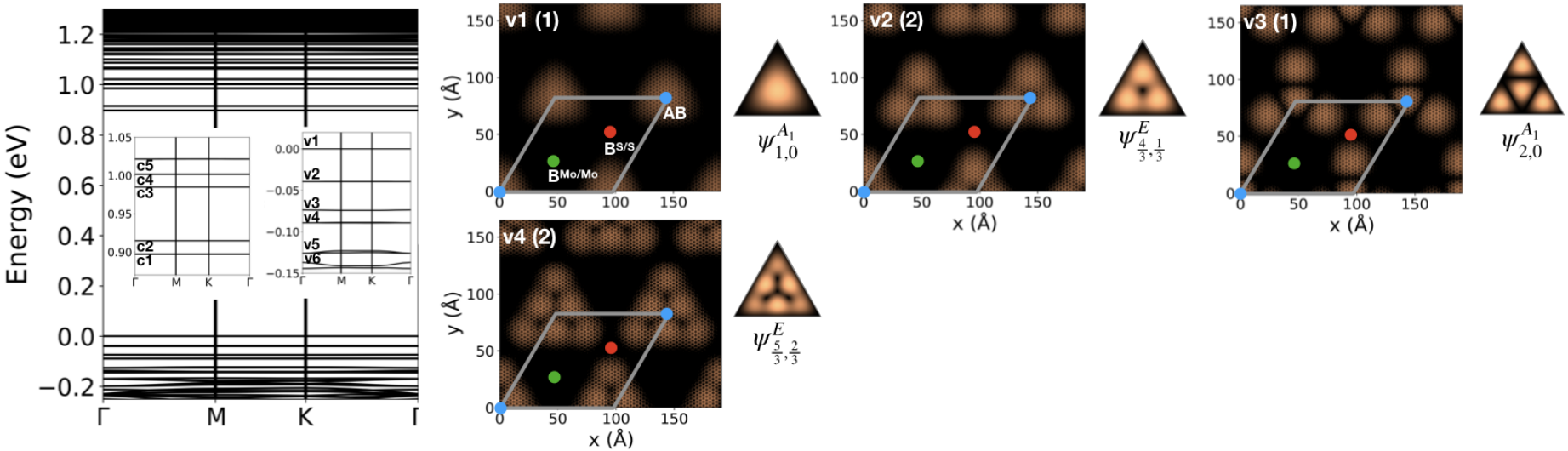
$\psi^{E}_{\frac{4}{3},\frac{1}{3}}$



$\psi^{A_1}_{2,0}$

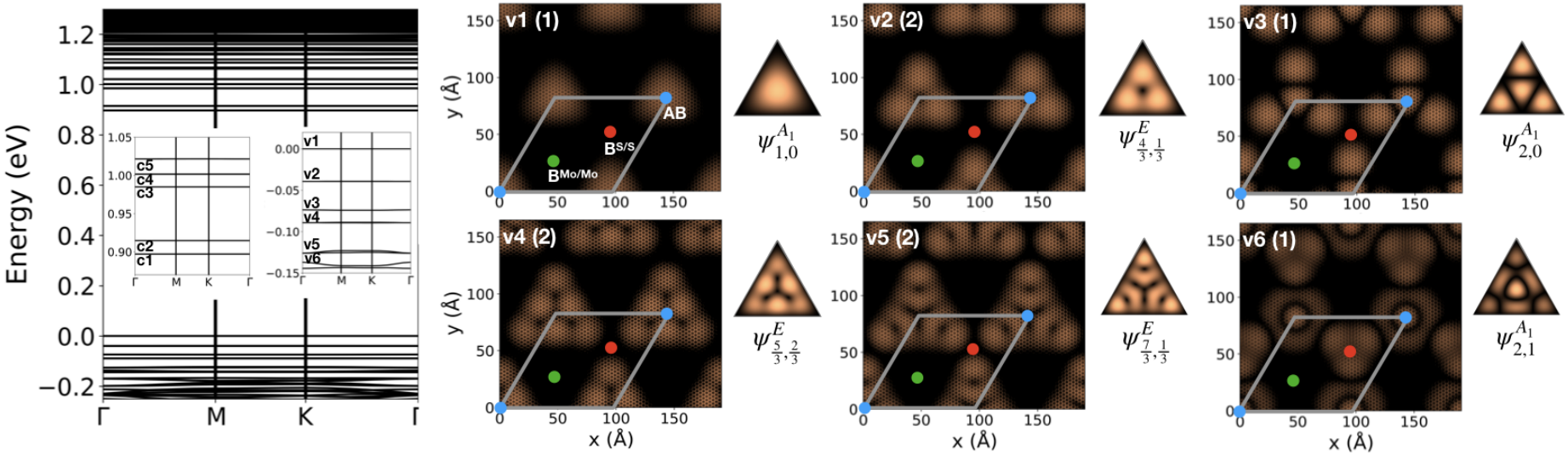
58° MSL

Equilateral triangle quantum well states.



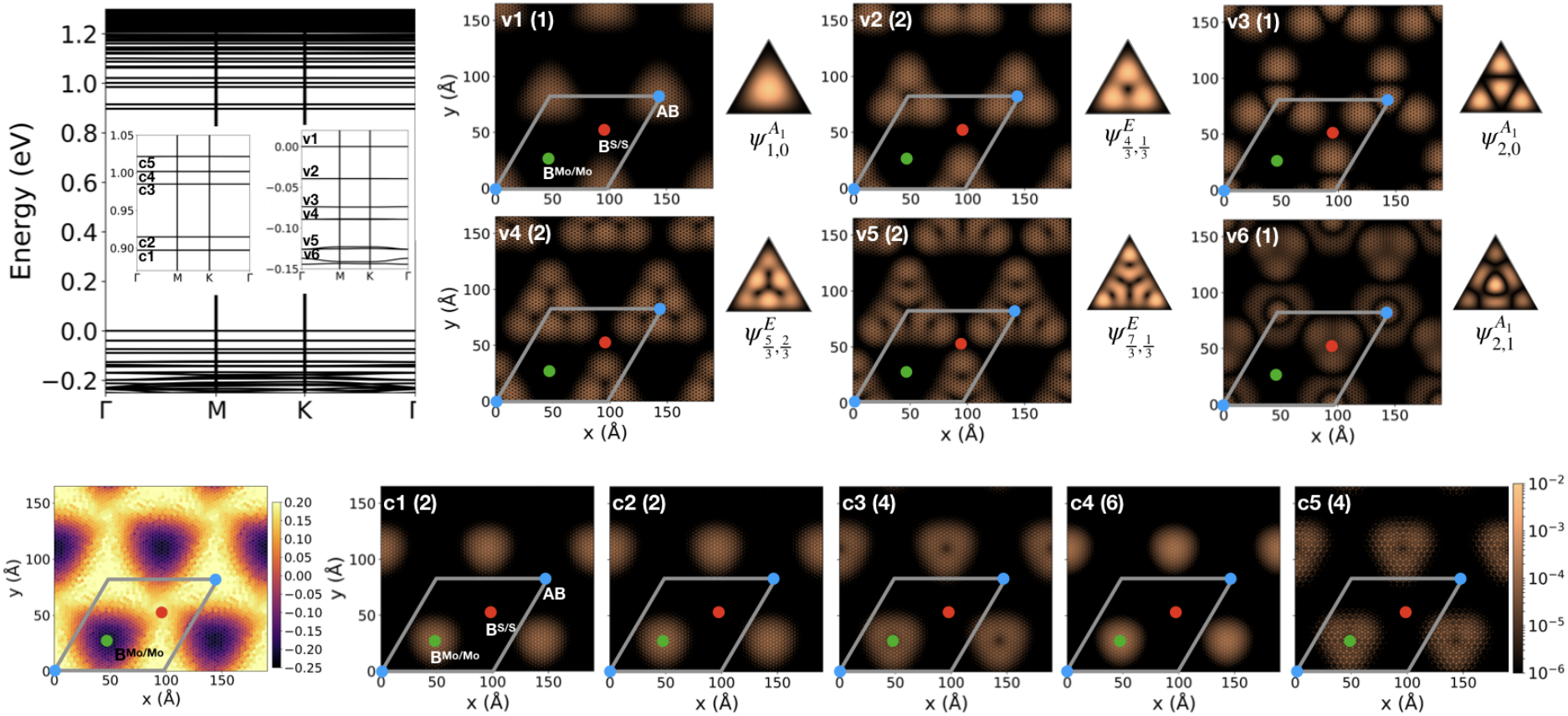
58° MSL

Equilateral triangle quantum well states.



58° MSL

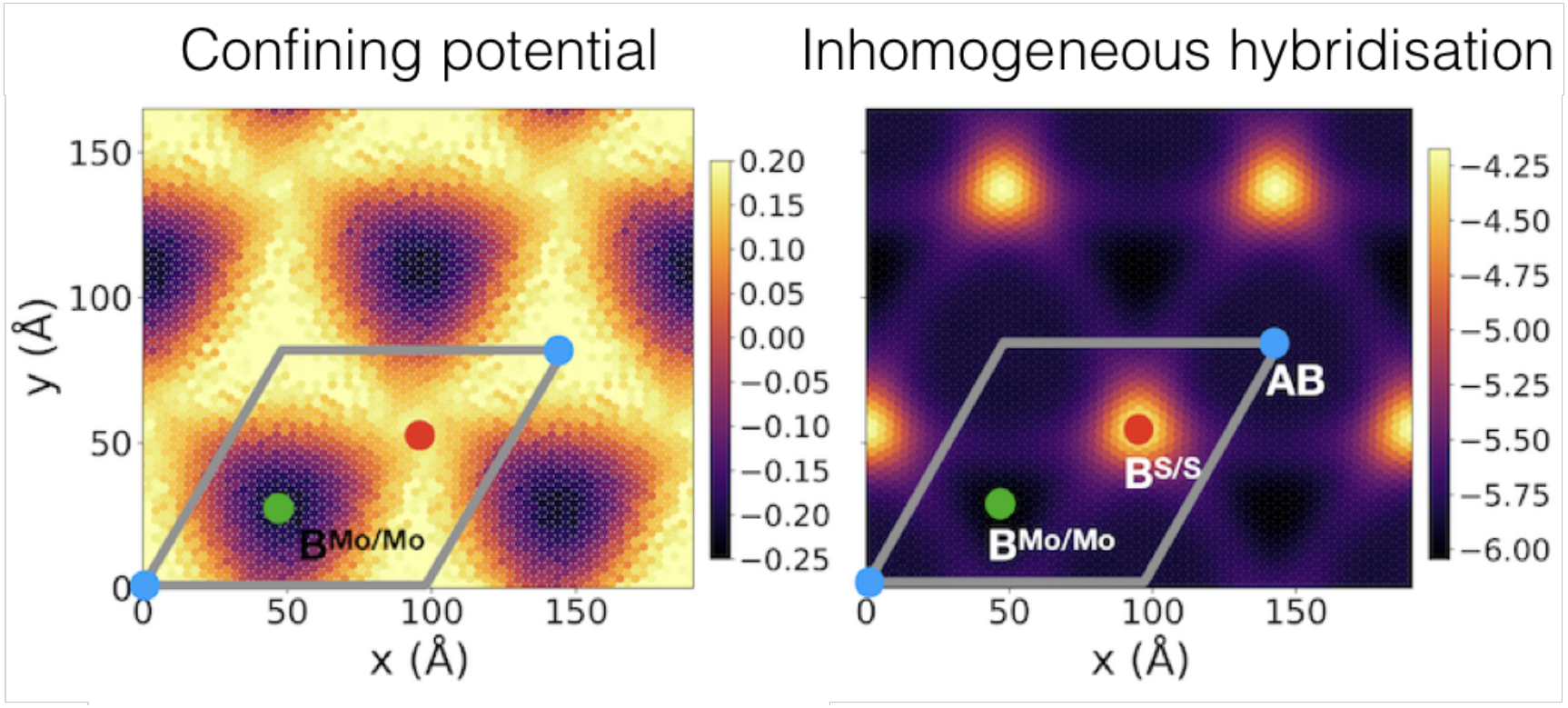
Equilateral triangle quantum well states.



Spatially separated electrons and holes.

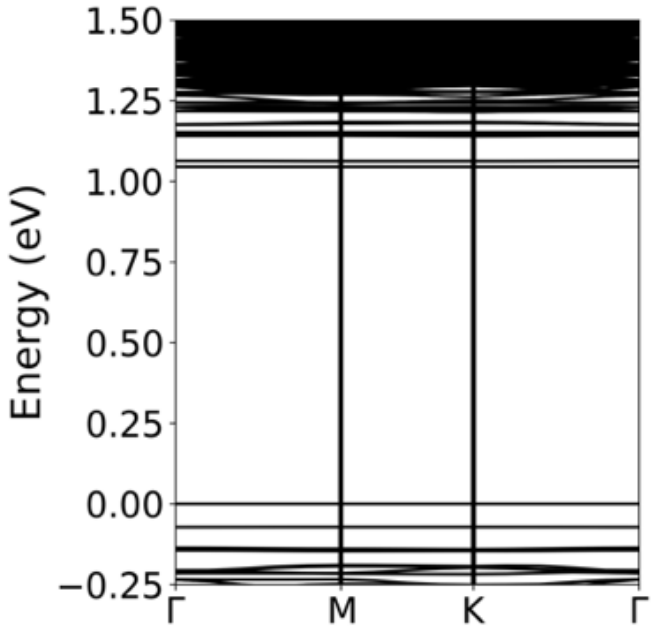
58° MSL: origin of localisation

Combined effect of inhmogeneous hybridisation and additional confining potential:



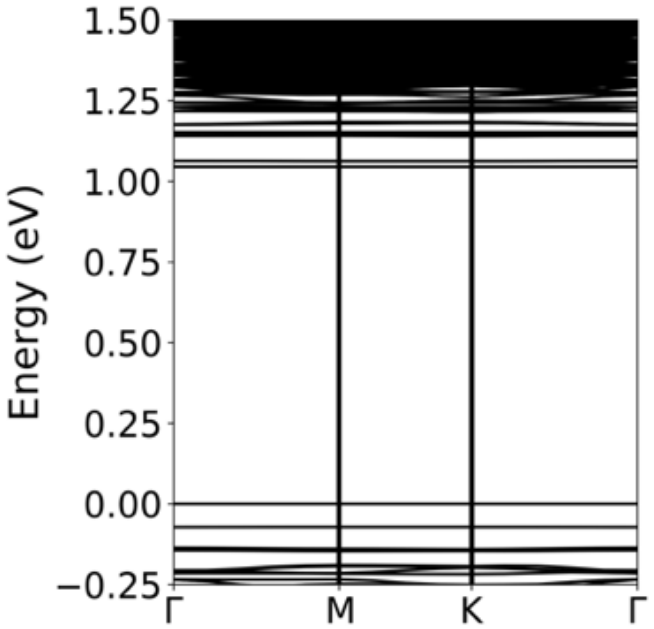
Effect of strains, 57.35° MSL

Relaxed structure
(including strains)

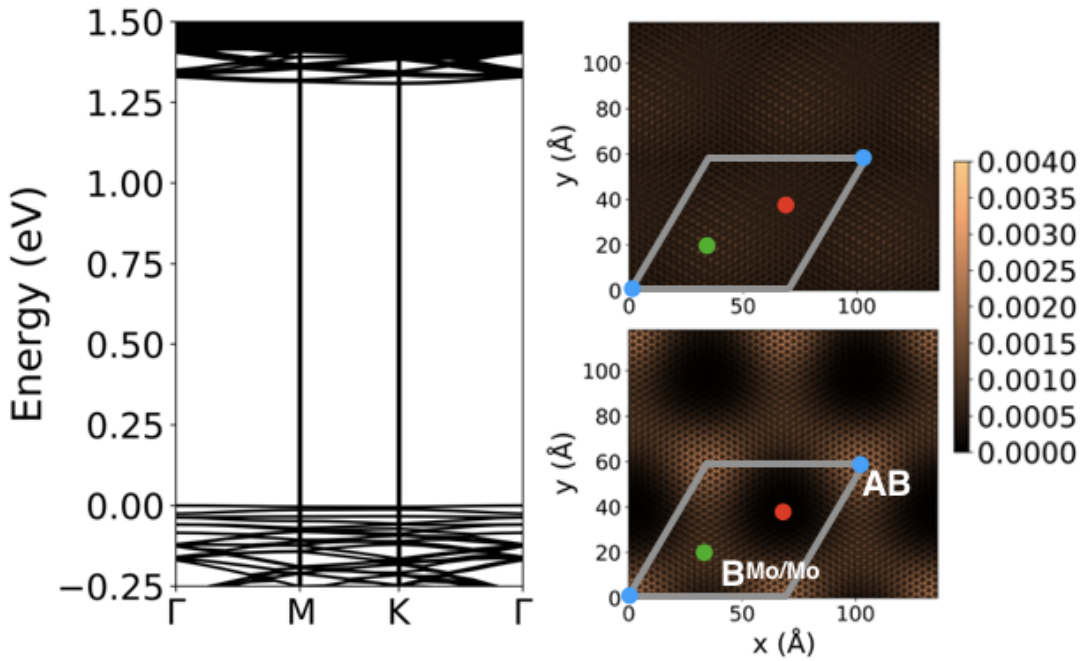


Effect of strains, 57.35° MSL

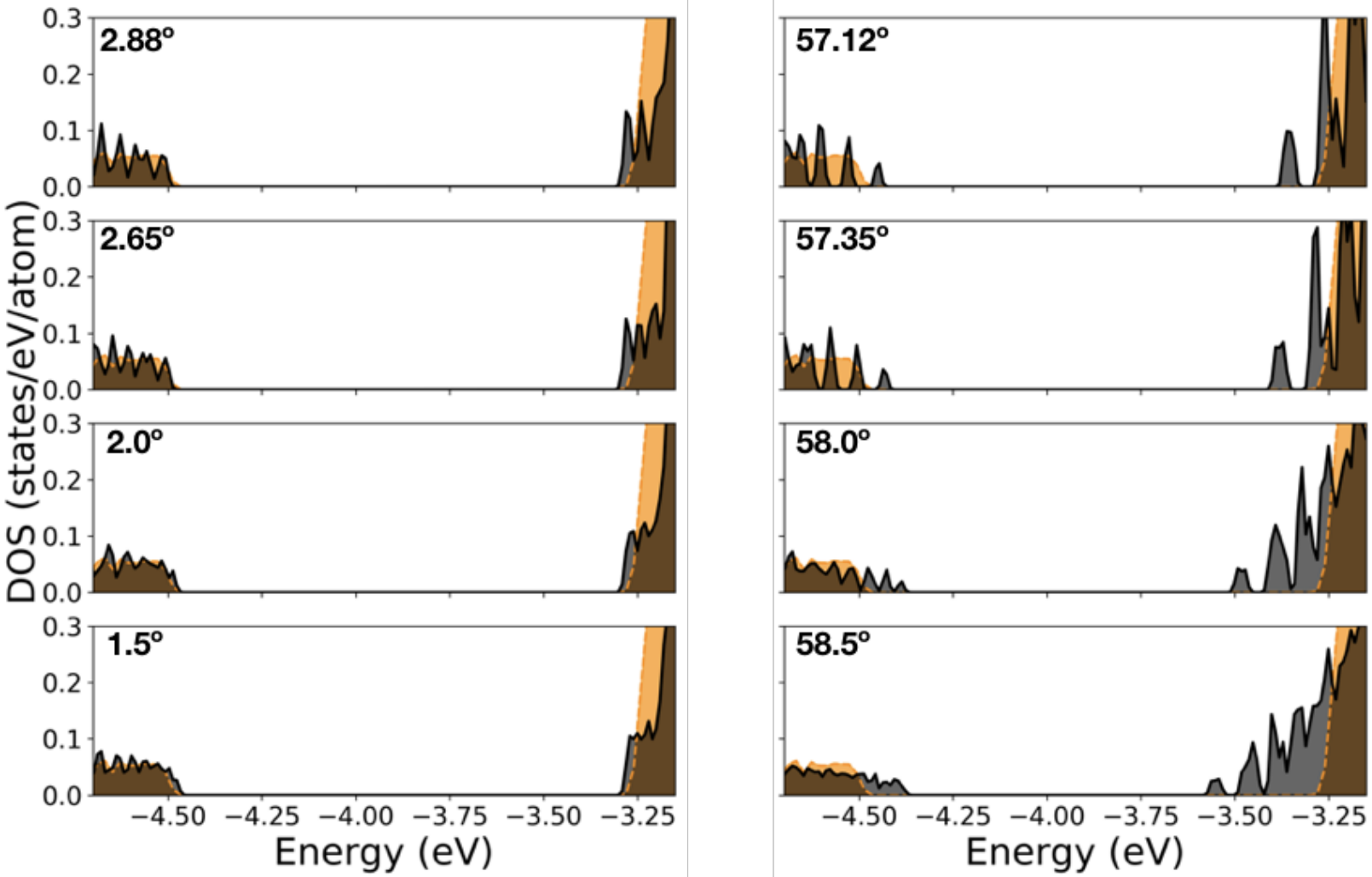
Relaxed structure (including strains)



Relaxed structure (excluding strains)



Density of states for twisted Moiré patterns



Conclusions

- We show that there are *no magic angles* in small-angle twisted bilayer MoS_2 and expect similar phenomenon in other TMD bilayers.

Mit H. Naik, Sudipta Kundu, Indrajit Maity and Manish Jain, arxiv:1908.10399.

Conclusions

- We show that there are *no magic angles* in small-angle twisted bilayer MoS_2 and expect similar phenomenon in other TMD bilayers.
- Demonstrate the formation of triangular quantum dots with spatially separated electrons and holes for twist angles close to 60°.

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Conclusions

- We show that there are *no magic angles* in small-angle twisted bilayer MoS_2 and expect similar phenomenon in other TMD bilayers.
- Demonstrate the formation of triangular quantum dots with spatially separated electrons and holes for twist angles close to 60°.
- Relaxations are crucial to get the correct picture for band localization – unrelaxed structures show spurious flatbands and localization.

Mit H. Naik, Sudipta Kundu, Indrajit Maity and Manish Jain, arxiv:1908.10399.

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Sudipta Kundu

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