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Impact of Relaxation Effects on Electronic and Transport Properties of Twisted Bilayer MoS_2

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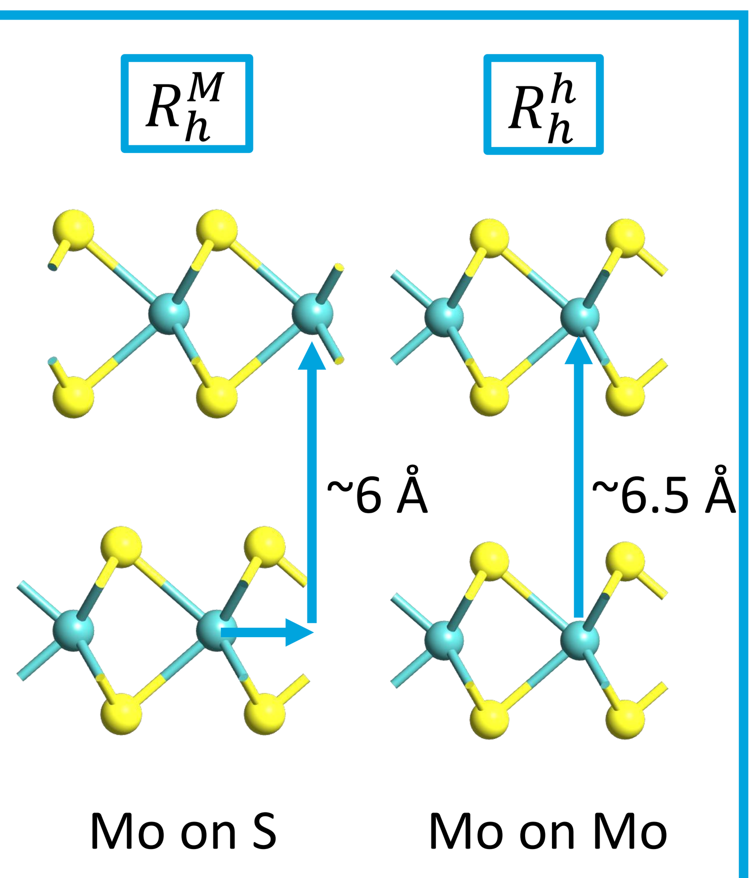
TECHNISCHE UNIVERSITÄT DRESDEN · HZDR · DRESDEN concept

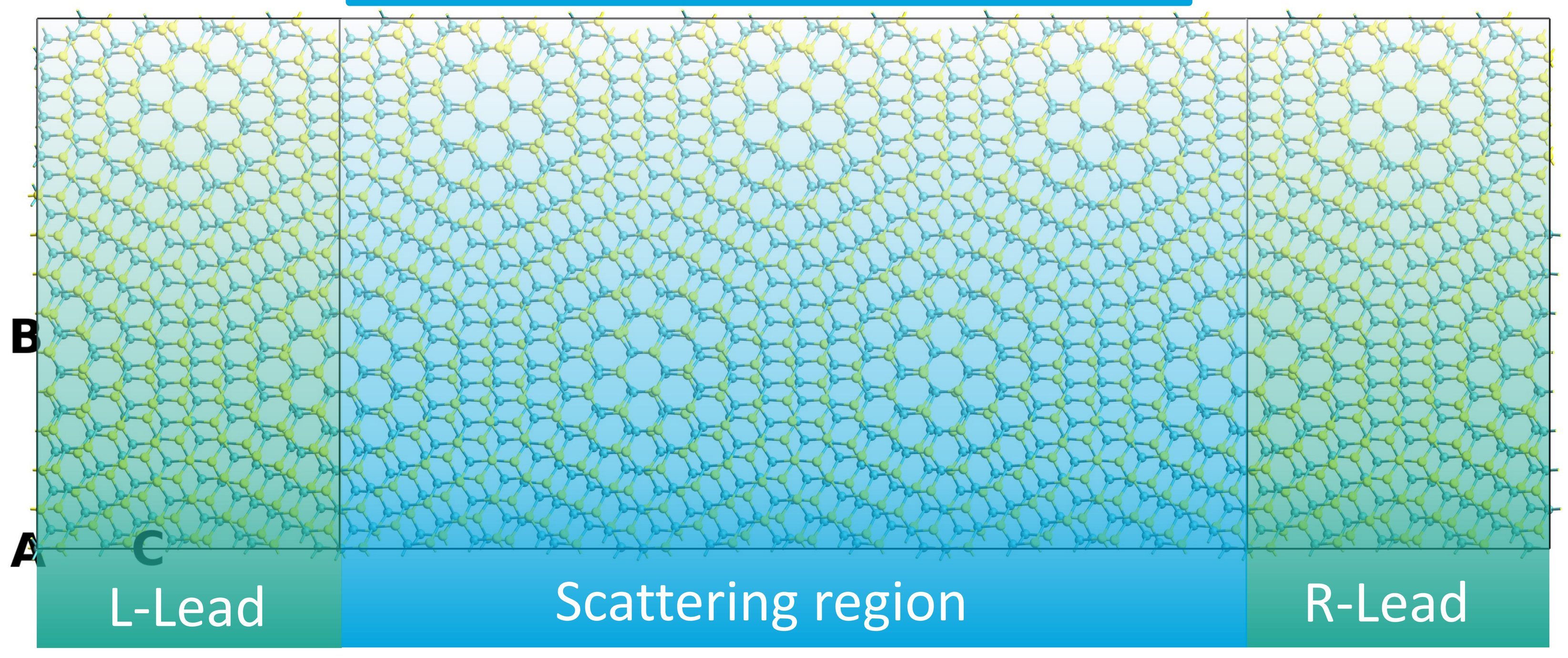
INTRODUCTION

Recent development in material science will push the new class of system explorations to the high-quality synthesis of 2D materials by mechanical and chemical exfoliation techniques. Hence, a new type of artificial crystals with novel electronic properties will emerge. Combining bilayers of 2D materials with a small twist angle leads to the formation of moiré superlattice, in which electronic properties can be tuned by changing twist angle θ.



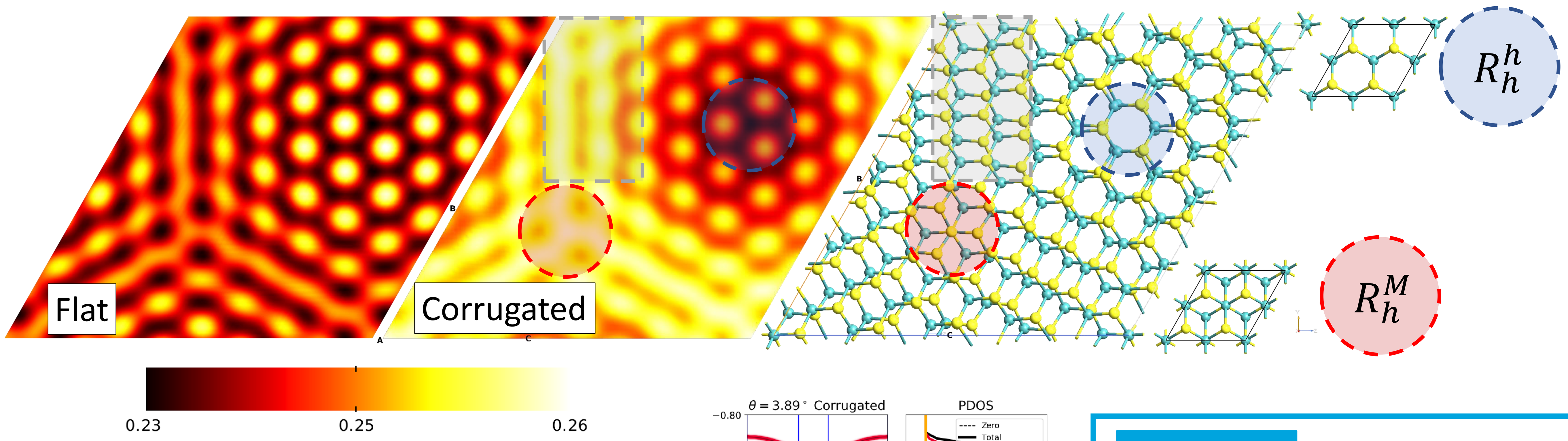
- The twisted bilayer MoS_2 with $\theta = 7.34^\circ$ is a semiconductor with transport gap of 1.69 eV (Corrugated) and 1.78 eV (Flat).
- Flat bands, sharp DOS, low velocity, electrons can not transport easily
- Dispersive (non-flat) bands, wide DOS, high velocity, rapidly moving electrons

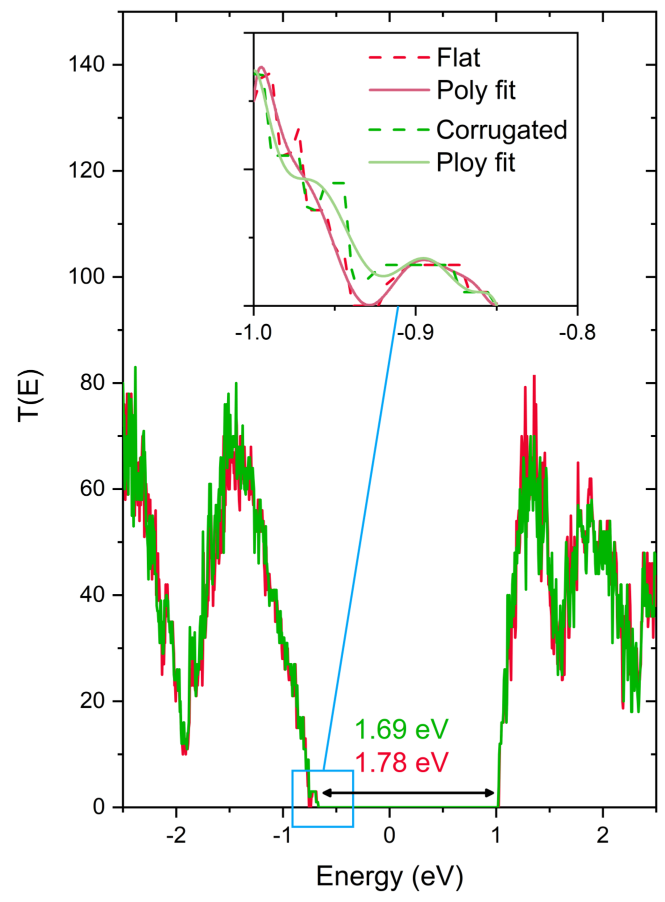
Device Configuration; $\theta = 7.34^\circ$



RESULTS

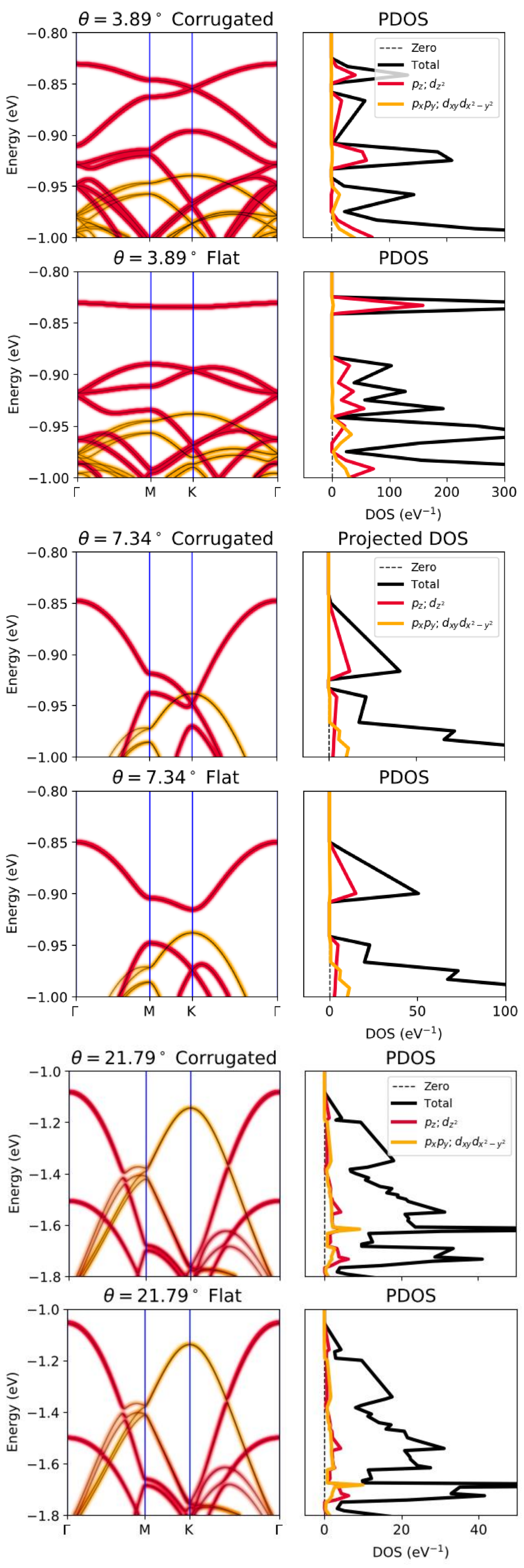
- The area of quasi- R_h^M domains in $\theta = 7.34^\circ$ increases after relaxation.
- The soliton is formed by atoms overlapped in zigzag manner, and uniform low-energy stacking R_h^M.

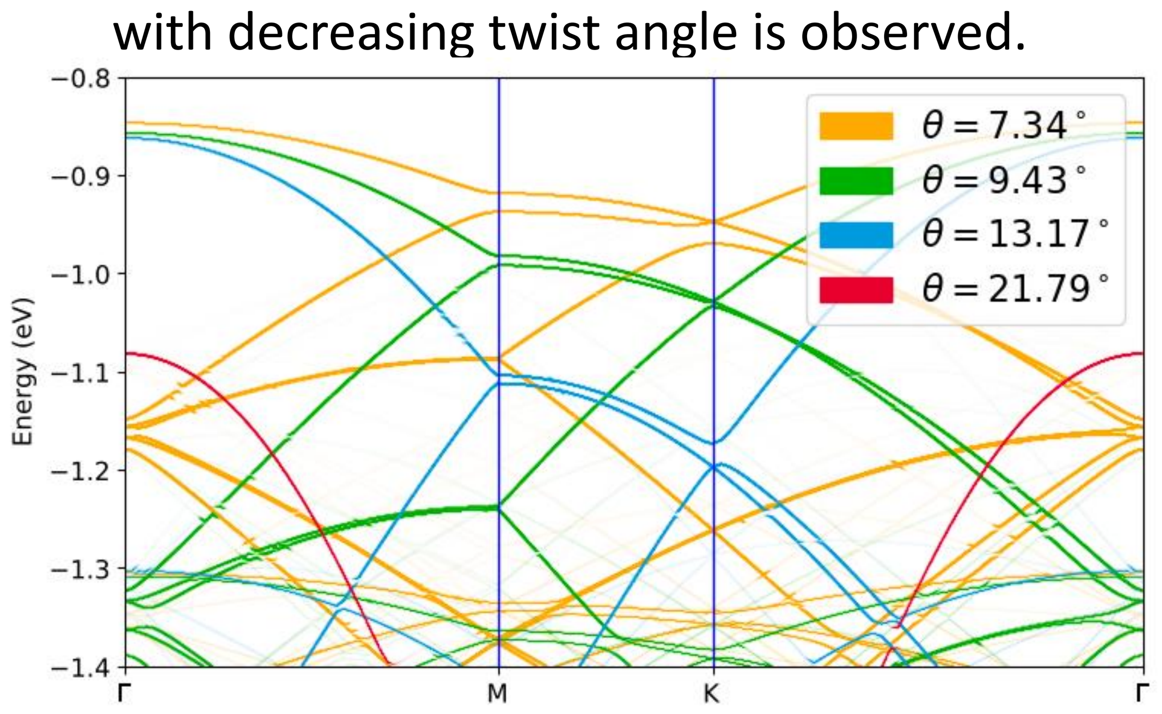


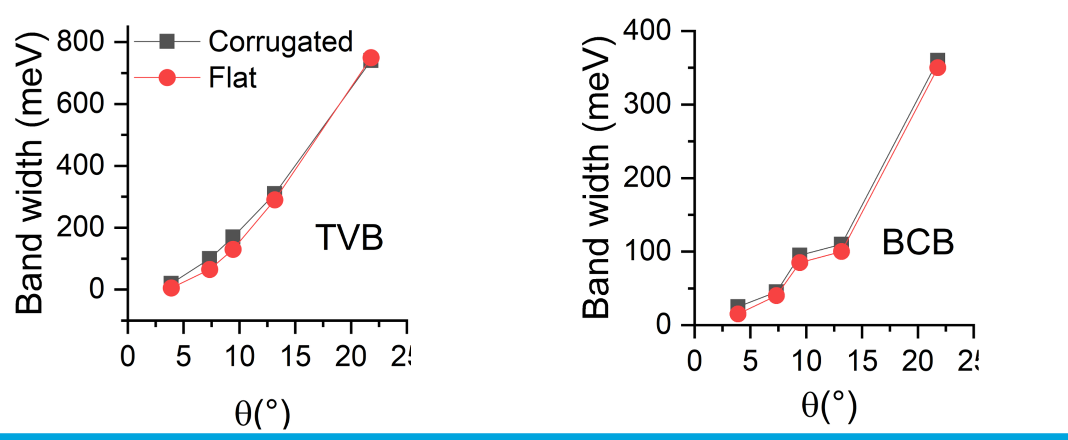


Transmission as function of energy for the above device configuration.

- The most spectacular effect of decreasing θ is the increase of the energies of some valence bands, thus gradually decreasing the gap.
- The evidence of solitons observed in the band structure for occupied states in $\theta = 7.34^\circ$ and 3.89°.
- Flat bands emerged for TVB (~5 meV) and BCB (~10 meV) in $\theta = 3.89^\circ$.
- A common trend of decreasing bandwidth with decreasing twist angle is observed.







METHODS

- Optimization was carried out thoroughly using the ReaxFF (Lattice vectors, and Atomic positions) by Ostadhossein et al [1].
- Density functional tight-binding model. Landauer-Büttiker formalism combined with non-equilibrium Green's function approach as implemented in QuantumATK 2019 package [2].
- Computational resources: ZIH
- Funding:

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SUMMARY

- Top Valence Band and Bottom Conduction Band evolve into flat bands at small twist angle with bandwidth smaller than 10 meV. The widths of flat bands can be controlled by moiré pattern.
- Flat valence band originates from the states around Γ point with both S p_z and Mo d_{z^2} characters.
- A 23 meV gap at the K point between p_z, d_{z^2} and $p_{xy}, d_{xy}\ d_{x^2-y^2}$ orbitals is existed, while hybridization may occur after structural relaxation in 7.34° sample.
- The emergence of a soliton in $\theta = 7.34^\circ$ and 3.89° have an influence on electronic properties.
- Structural relaxation have an influence on the topology of valence bands, which a Dirac node, confirm honeycomb picture in $\theta = 3.89^\circ$.

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