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Reconstruction of moiré lattices in twisted transition metal dichalcogenide bilayers

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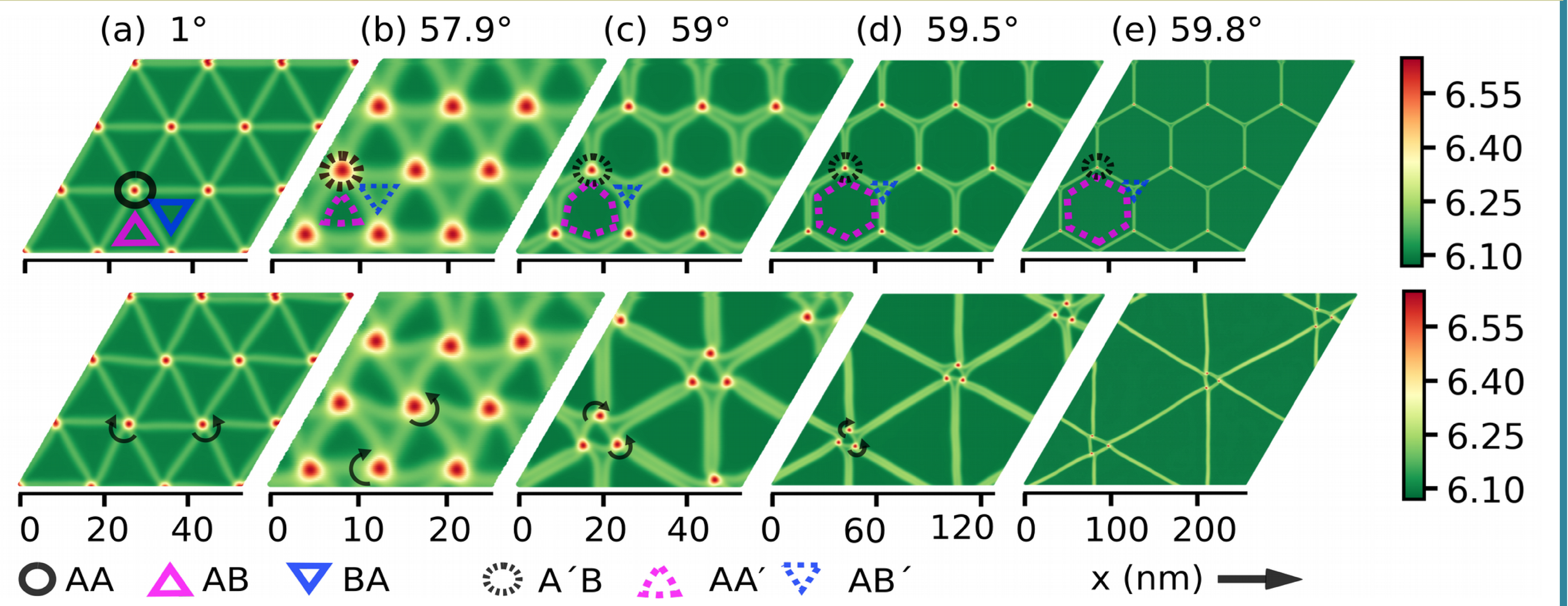
Introduction

- Moiré patterns created with transition metal dichalcogenides can host correlated electronic phases, long-lived excitons, phasons.
- An important step to understand the novel electronic, optical, and vibrational properties is the incorporation of structural relaxation effects.
- To date, all studies conducted on moiré patterns presume that the moiré lattice constant before and after relaxation are identical.

Questions addressed

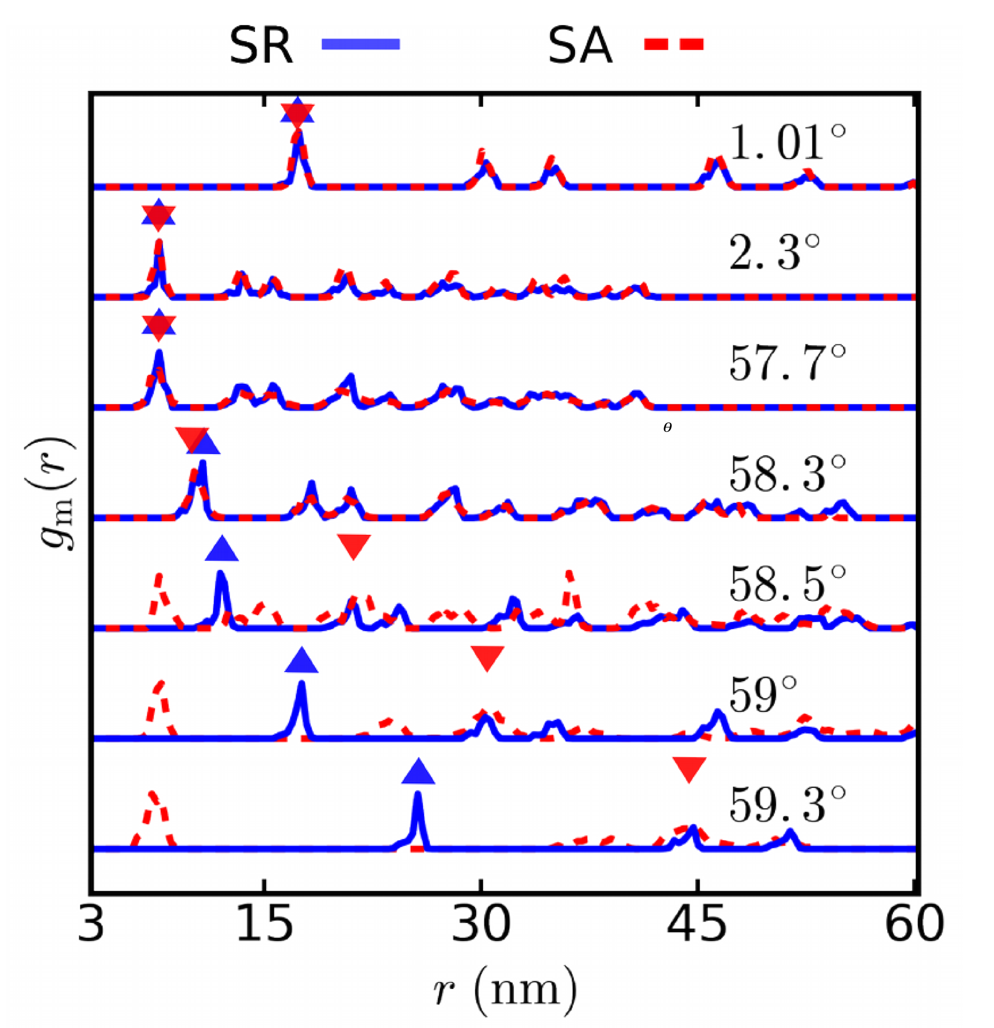
- Can there be novel lattice reconstruction?
- What are the consequences of such reconstruction on electronic properties ?

Dramatic reconstruction of moiré lattices with simulated annealing



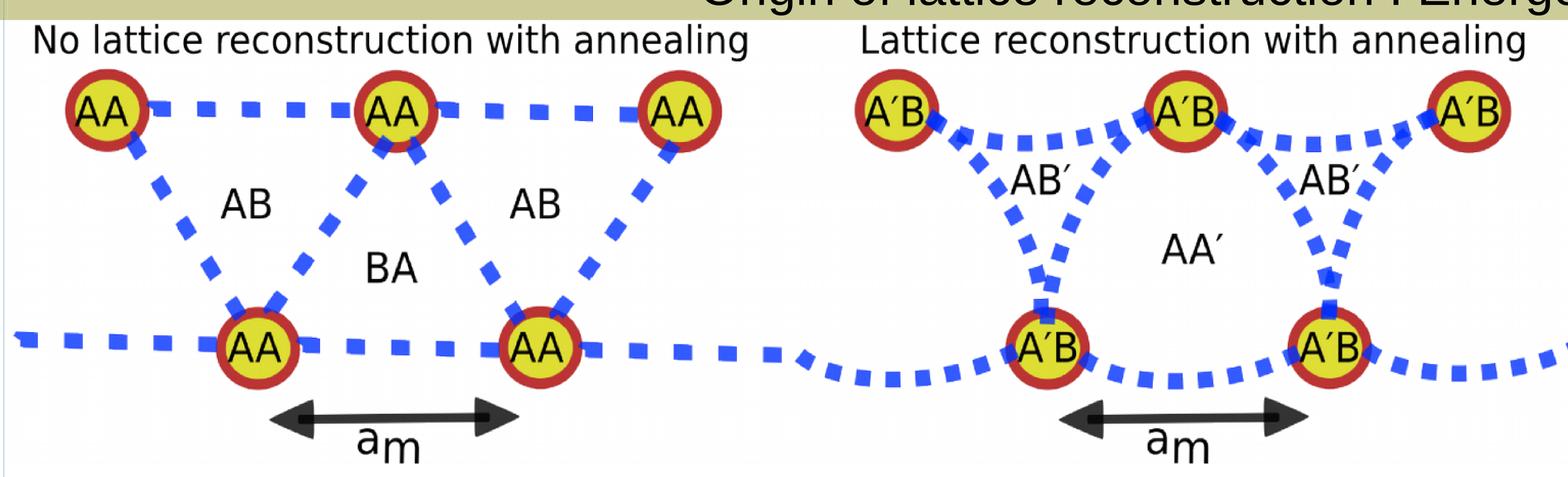
(a)-(d): Interlayer separation of twisted bilayer MoS_2 using standard relaxation (top panel) and simulated annealing (bottom panel). The smallest repetitive cell in the top panel is a moiré unit cell. The scales of the colorbar, in Å and corresponds to interlayer separation. The curling of domain walls near a few AA, AB´ stackings are marked.

Long-range order of the moire lattices



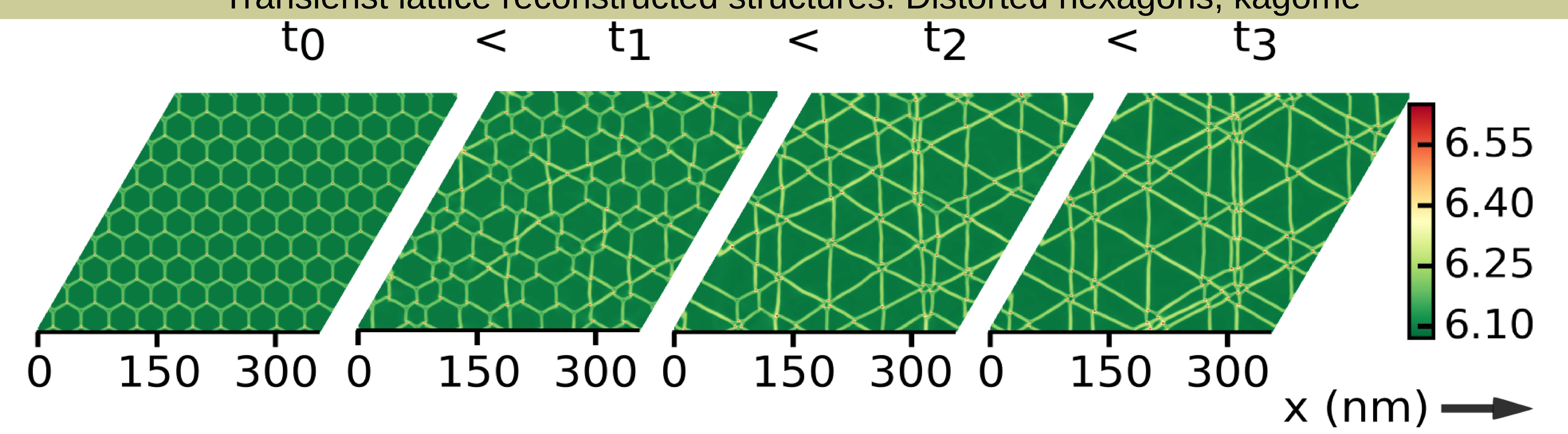
- Radial distribution function at moire scale, $g_m(r)$ using both standard relaxation (SR) and simulated annealing (SA).
- Evidence of lattice reconstruction as $\theta > 58.4^0$

Origin of lattice reconstruction : Energetics



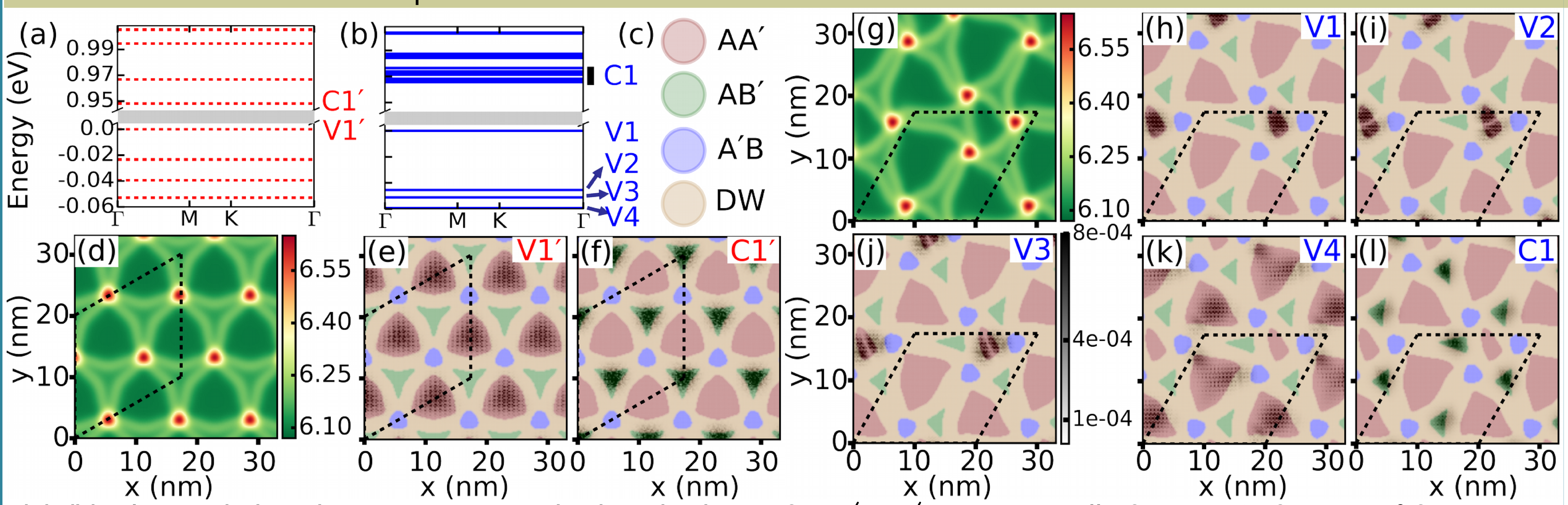
- Total energy measured with respect to stable stacking is ∝ length of the domain wall (dashed lines) and repulsive.
- Lattice reconstruction occurs to minimize the length of domain walls.

Transienst lattice reconstructed structures: Distorted hexagons, kagome



- Examples of other possible transient structures found with simulated annealing (SA) which can be metastable in experiments.

Impact of lattice reconstruction on electronic band structure



(a),(b) Electronic band structures near the band edges of a $\sqrt{3}x\sqrt{3}x1$ supercell of $tBLMoS_2$ for 58.47⁰ for un-reconstructed and lattice reconstructed structures, respectively. The supercell is marked with black dashed lines in (d),(g), respectively. (c) Colors used to denote stackings in (e)-(f),(h)-(l). $|\psi_r(r)|^2$ of the states near valence band maximum, and near conduction band minimum for structures obtained with SR ((e)-(f)) and with SA ((h)-(l))

Conclusions

- The presumption that the moiré lattice constnat of the rigidly twisted structure continues to characterize the relaxed twisted structure is in general invalid.
- The lattice reconstruction significantly modifies the electronic band structure.
- These lattice reconstruction for small twist angles near 60⁰ is generic to any transition metal dichalcogenides and their heterostructures.
- Multiple flat-bands can host a rich variety of correlated electronic phases.

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References:
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2. I. Maity, M. H. Naik, P. K. Maiti, H. R. Krishnamurthy, M. Jain, Phys. Rev. Research 2, 013335 (2020)

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