Reconstruction of moire lattices in twisted transition metal dichalcogenide bilayers

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The introduction of a small twist angle (θ) between two layers of two-dimensional materials gives rise to a large-scale lattice (moiré), which can significantly alter its structural, electronic and vibrational properties. An important step in understanding these properties of the moiré lattices is the inclusion of the effects of structural relaxation of the un-relaxed twisted structures. Here, we propose new candidate structures for twisted bilayer of transition metal dichalcogenides (TMDs). For θ > 58.4°, we find a dramatic reconstruction of the moiré lattices. The moiré lattice constant of the reconstructed structure is √3 times that of the un-relaxed twisted structure. We show that the development of curved domain walls due to the three-fold symmetry of the stacking energy landscape is responsible for such reconstruction.

References

[1] I. Maity, P. K. Maiti, H. R. Krishnamurthy, M. Jain, *arXiv preprint arXiv:1912.08702*
[2] I. Maity, M. H. Naik, P. K. Maiti, H. R. Krishnamurthy, M Jain, *arXiv preprint arXiv:1905.11538*

Figures

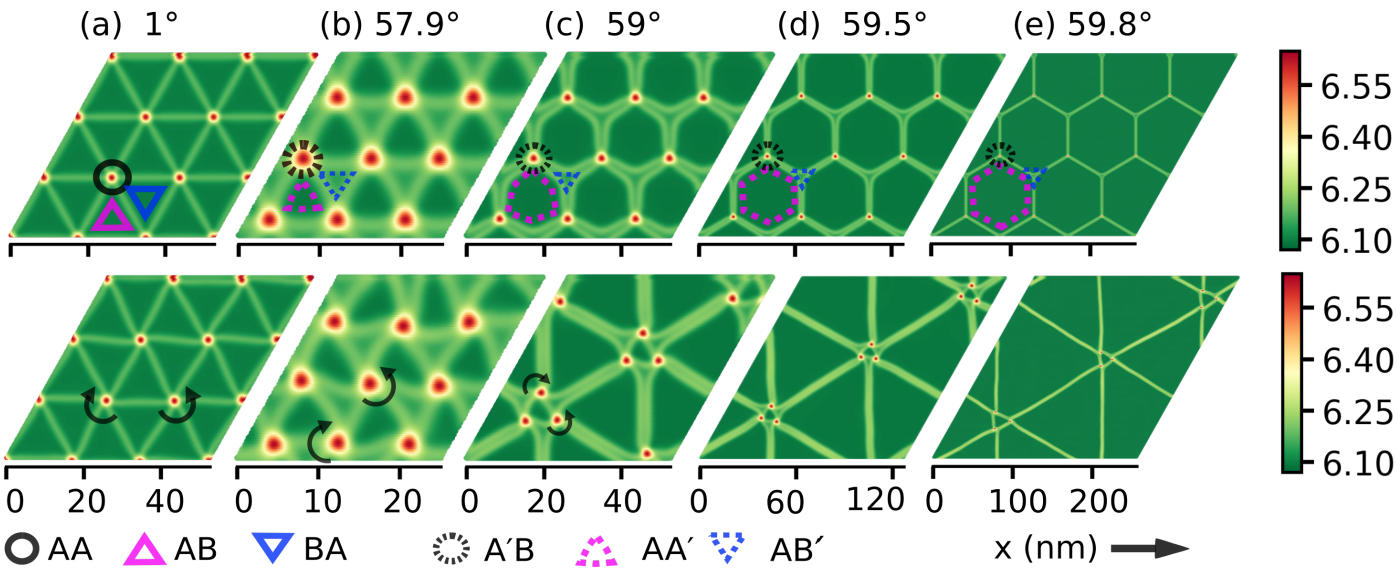

Figure 1: Interlayer separation landscape using standard relaxation (top panel) and simulated annealing (bottom panel) for tBL of MoS_2 (using Mo atoms). The smallest repetitive cell in the top pannel is a moiré lattice. The scales of the associated colorbar are in Å and denotes interlayer separation.