Structural properties of twisted transition metal dichalcogenides heterobilayers

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Abstract

Introducing an interlayer twist angle in bilayers of two-dimensional (2D) graphene resulted in new and unexpected physics [1]. Despite the absence of strong interlayer interactions, the twist angle and the stacking domain formation due to relaxation, determine the properties of these twisted bilayers. Also 2D crystals beyond graphene, such as transition metal dichalcogenides (TMDCs), show enhanced electronic correlations that are affected by twisting [2]. Furthermore, due to different lattice constants, heterobilayers result in moiré structures even without twist. Yet, the atomic structure of twisted TMDC heterobilayers is not explored thoroughly due to the large computational cost resulting from the moiré cells which typically include many thousands of atoms. Therefore, here, we systematically explore the structure of group 6 TMDC heterobilayers consisting of MoS_2, WS_2, $MoSe_2$ and WSe_2 monolayers as function of the interlayer twist angle. We find for all systems significant lattice reconstruction, involving in- and out-of-plane relaxations, which strongly depends on the twist angle. We can categorize the results in two principal cases: at large twist angle, the two constituting layers exhibit little adjustment; at small twist angle, the high-energy stacking regions shrink, while low-energy ones expand, forming multiple domains with matching lattice constants which are separated by boundaries. In particular, the two constituting layers show significant asymmetrical corrugation. We reveal that the lattice reconstruction results from the competition between strain energy cost and van der Waals energy gain. These superstructures with domains of different local stacking suggest intriguing electronic properties intriguing electronic properties of these systems.

References

[1] R. Bistritzer and A. H. MacDonald, Proc. Natl. Acad. Sci. 30 (2011), 12233.
[2] Z. Zhang *et al.*, Nat. Phys. 11 (2020), 1093.

Figures

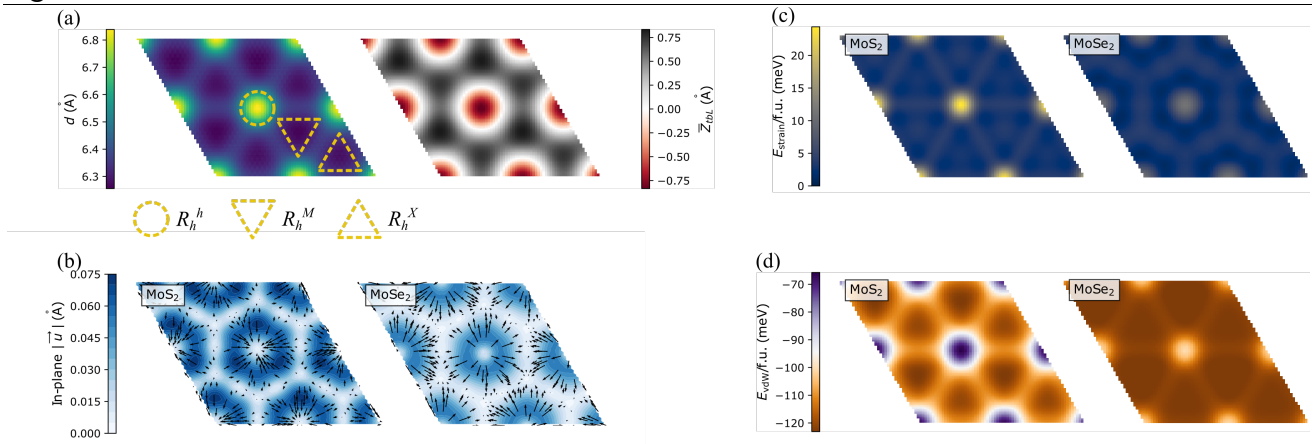

Figure 1: In $MoS_2/MoSe_2$ heterobilayers at θ = 0°, distribution of (a) Interlayer distance *d*, average out-of-plane displacement $\overline{Z}_{tbL}$, and (b) in-plane displacement of metal atoms in each constituting layer. (c) Calculated strain energy and (d) vdW energy of all atoms in each constituting layer.

out-of-plane displacement $\bar{\mathbf{Z}}_{\mathbf{tbL}'}$ and (b) in-plane displacement of metal atoms in each constituting layer. (c) Calculated strain energy and (d) vdW energy of all atoms in each constituting layer.