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Atomic reconstruction in twisted transition metal dichalcogenide heterostructures

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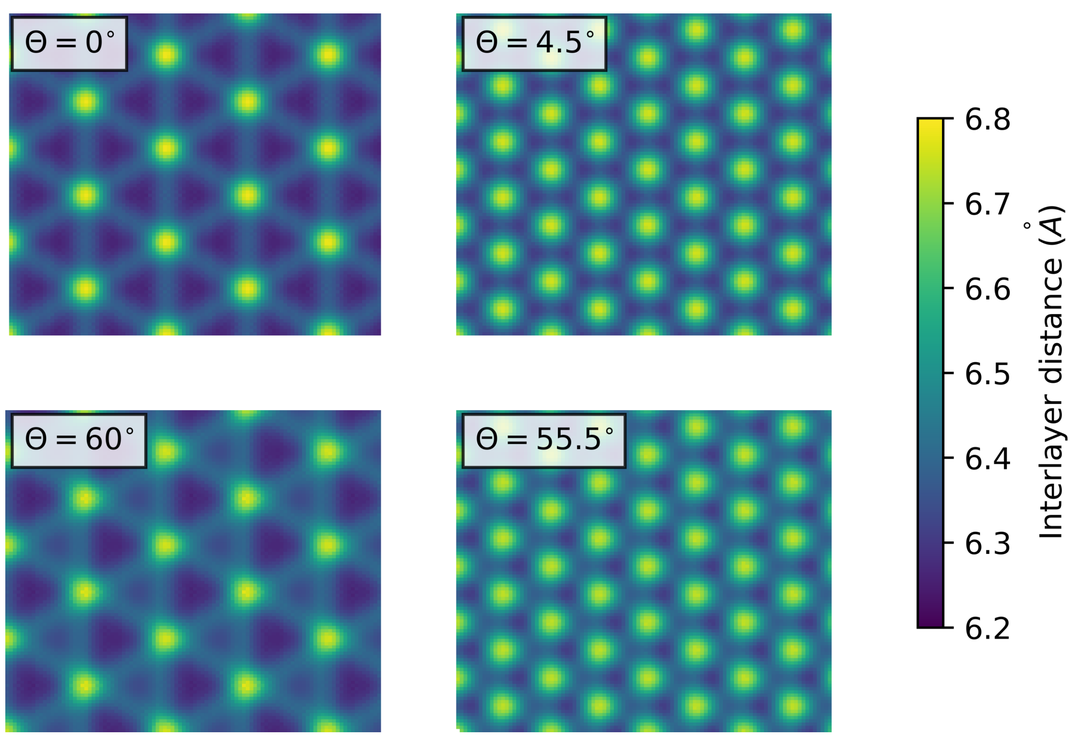
Introduction

The interlayer van der Waals (vdW) interactions enable two single layers of a two-dimensional material to vertically stack together and form van der Waals heterostructures (vdWHs). If the two layers have different distinct symmetries or lattice sizes or if they are twisted with respect to each other, a moiré pattern with much larger length scale than the periodicity of each layer is formed. The moiré superlattice can be further modified by twist angle, which means moiré superlattice is also formed in twisted homostructures. As moiré patterns deeply alter the physical properties of bilayer systems, the controllable design of twisted heterostructures clearly allows for new physics and engineering directions. In this case, lattice reconstruction will be vital for further understanding electronic and optical properties of these complicated moiré interfaces.

Result

- Domain formation in large-size cell
- Also observed in twisted bilayer graphene[2] and graphene/h-B heterostructures[3].



- Domain accumulate the generated strain

Method

- Force-field method[1] employing the Stillinger-Weber (SW) and Kolmogorov-Crespi (KC) potential
- Standard energy minimization and classical molecular dynamics simulations using LAMMPS
- Interpolated interlayer distance and displacement
- Computational resources: ZIH
- Funding:

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- Significant out-of-plane deformation

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