Structural and electronic properties of twisted MoS_2 bilayers

Viet-Anh Tran
Viet-Hung Nguyen, Jean-Christophe Charlier
University of Louvain (UCLouvain), Institute of Condensed Matter and Nanosciences, Louvain-la-Neuve, Belgium
anh.tran@uclouvain.be

2D layered structures of transition metal dichalcogenides (TMDCs) such as molybdenum disulfide (MoS_2) are attracting increasing attention due to their rich and tunable electronic properties [1]. In analogy to the well-known twisted graphene-based systems, when MoS_2 layers are stacked with a relative twist, a moiré superlattice is formed, inducing new interlayer coupling which significantly modifies the corresponding electronic structure [2]. The twist angle between MoS_2 layers can strongly influence both the band gap and the emergence of flat bands at small angles, allowing the exploration of correlated electronic states and novel quantum effects [3]. In addition, atomic reconstruction occurring in small twist-angle moiré structures substantially alters the band structure, further enriching their electronic properties [4]. Despite rapid progress, a comprehensive understanding of how the twist angle governs these electronic properties remains an open question. In this work, atomistic modelling approaches, including tight-binding calculations and molecular dynamics simulations, are used to systematically investigate the influence of the twist angle on both structural and electronic properties of twisted MoS_2 bilayer.

References

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[3] L. Xian et al., Nat. Commun. **12** (2021), 5644
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Figures

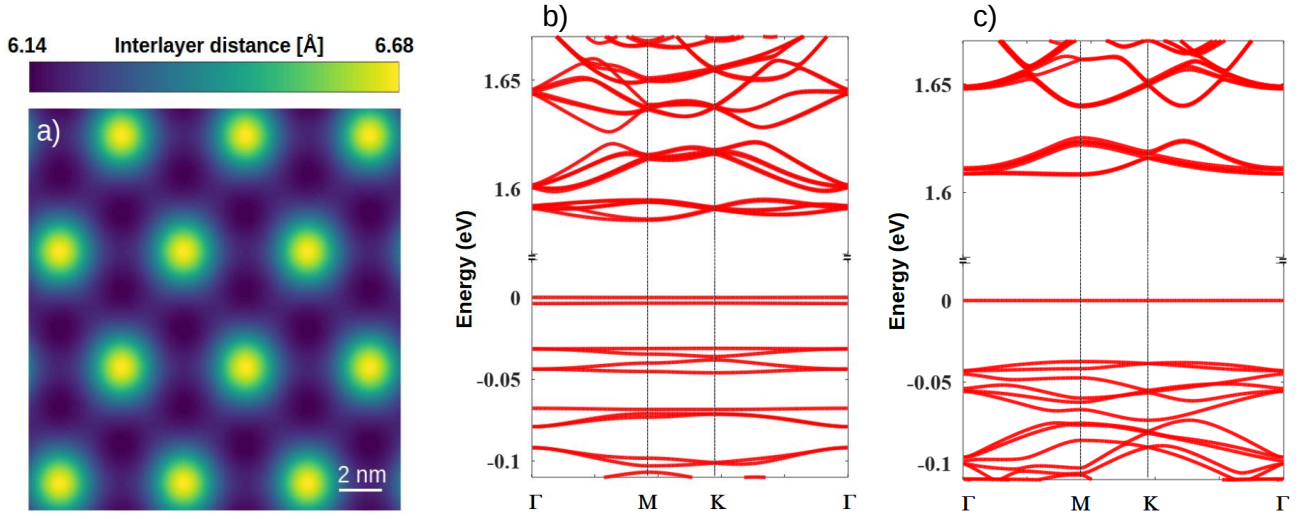

Figure 1: Moiré superlattices arising in twisted MoS_2 bilayer system. (a) Spatial map of interlayer distance(corrugation) in 3.15° twisted MoS_2 bilayer (b,c) Electronic band structure of 3.15° twisted MoS_2 bilayer with and without structural relaxation, respectively.