Moiré metrology of energy landscapes in van der Waals heterostructures

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The emerging field of twistronics has revolutionized quantum materials research. At the small twist limit, and particularly under strain, as atomic relaxation prevails, the emergent moiré superlattice encodes elusive insights into the local interlayer interaction. In this work we introduce moiré metrology as a combined experiment-theory framework to probe the stacking energy landscape of bilayer structures at the 0.1 meV/atom scale, outperforming the gold-standard of quantum chemistry. Through studying the shapes of moiré domains with numerous nano-imaging techniques, and correlating with multi-scale modelling, we assess and refine first-principle models for the interlayer interaction. We document the prowess of moiré metrology for three representative twisted systems: bilayer graphene, double bilayer graphene and H-stacked $MoSe_2/WSe_2$. Moiré metrology establishes sought after experimental benchmarks for interlayer interaction, thus enabling accurate modelling of twisted multilayers.

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