

Impact of Twist Angle on Electronic Transport Properties of Bilayer MoS₂

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Tuning the twist angle between adjacent layers of two-dimensional semiconductors (2DS), to control the topology and interlayer interactions, offers an additional degree of freedom, which facilitate optical, mechanical, and electronic properties different than in the untwisted case. Twisted 2D crystals result in a moiré pattern, where lattices of the 2D material form a superlattice, which would bring well-defined positioning and changes in the behavior of electrons in the material. To understand the application of twistronics, it is crucial to control the interlayer twist angle on a large scale.

In this study, we performed density-functional-based tight-binding calculations combined with Landauer- Büttiker formalism and non-equilibrium Green's function approach to study electronics of twisted bilayer MoS₂ and to analyze the impact of twist angles on transport properties.

Twisted MoS₂/MoS₂ model shows slightly changes in transmission as function of energy when compared with the untwisted systems. Furthermore, we show a comprehensive overview of the impact of twist angle, ranging from 0° to 40°, on the ballistic transport for both flat and corrugated twisted bilayer MoS₂. An example is shown in Figure 1.

Figures

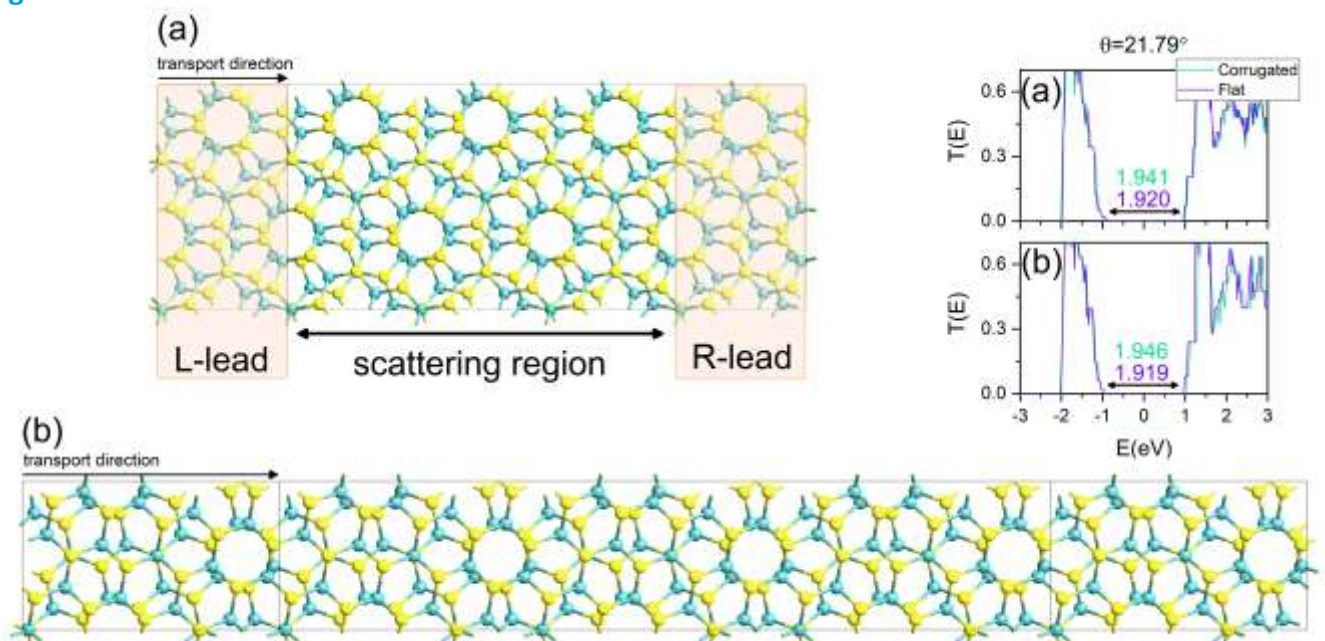


Figure 1: Schematic representation of MoS₂/MoS₂ device configuration and corresponding transmission as function of energy along *a* and *b* directions.