UNFOLDING
THE ELECTRONIC BANDS OF TWISTED 2D MATERIALS

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Two-dimensional (2D) heterostructures can be very effectively built by direct stacking of individual monolayers of different 2D materials. The extended range of functionalities of such heterostructures yields possible applications going from field effect tunneling transistors to optoelectronic devices. In order to control the ultimate performance of these systems it is fundamental to understand how the electronic properties of each layer are affected by the neighboring one. These effects can be reliably described in the framework of the Density Functional Theory (DFT) but the electronic structure derived from a moiré supercell model results in highly folded bands, which can be hardly linked to those of the reference unstacked lay that which provide an effective band structure, which has great interpretative value and can help for instance in the understanding of angle-resolved photoemission spectroscopy (ARPES) measurements.

As an example, here we show how band unfolding can correctly describe the appearance of additional gaps in the electronic structure of MoS_2 on top of black phosphorous which has been observed by ARPES. Band unfolding techniques have been further applied to the study of bilayer moiré structures of emergent optical materials such as BN and WSe_2. After discussing the dependence of the electronic structure on the twist angle, we combine this ground state information with simulations of the optical response obtained by a GW+BSE approach. Finally we discuss how the twist of the layers can affect the excitonic response of the bilayers.

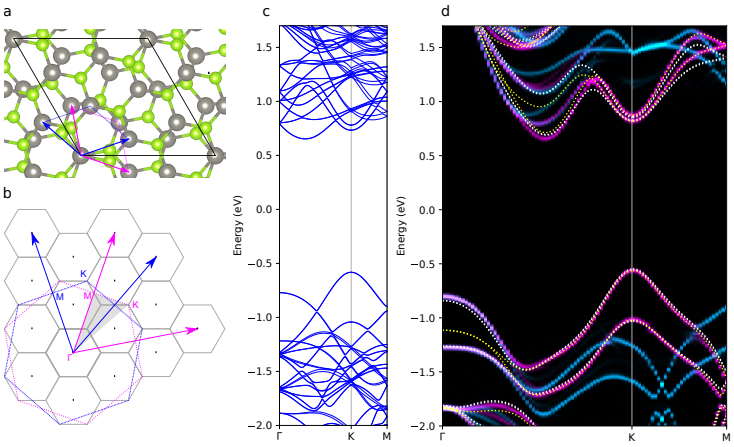

Figure 1: a) Structure of a moiré WSe2 supercell where the primitive unit cell of the top and bottom layer are indicated. (b) Reciprocal lattice vectors and Brillouin zones of the primitive cells of the individual layers, and the supercell Brillouin zones (grey hexagons). (c) Band structure calculated over the high symmetric direction of the moiré supercell. (d) Band structure of the moiré cell unfolded along the high symmetry direction of the reduced Brillouin zone shaded in (b). Blue and purple lines correspond to the unfolding using the reference primitive cell of the top and bottom layer respectively. The yellow and white lines are the band structure of WSe2 mono- and bi-layer respectively.

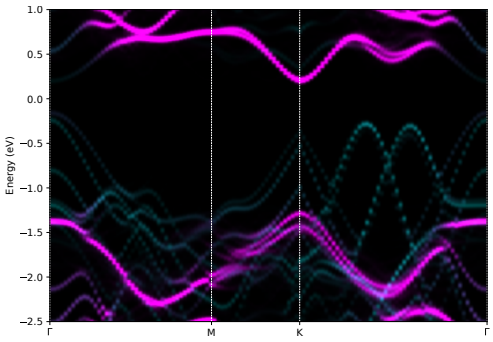

Figure 2: Electronic band structure of a stack of monolayer MoS_2 on top of black phosphorous unfolded using as reference the MoS_2 (purple lines) and the black phosphorous (cyan lines) primitive cells.

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