UNFOLDING

THE ELECTRONIC BANDS OF TWISTED 2D MATERIALS

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Two-dimensional heterostructures can be built very efficiently by directly stacking individual monolayers of different 2D materials. Their wide range of functionality allows for applications spanning from tunneling transistors to optoelectronic devices. In order to control the final 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 within the framework of density functional theory (DFT), but the electronic structure derived from an extended supercell moiré model results in highly folded bands, which are difficult to relate to those of the reference non-stacked layers. This complication can be overcome by using unfolding methods that provide an effective band structure, which has great interpretive value. Band unfolding can help in understading angle-resolved photoemission spectroscopy (ARPES) but also other spectroscopic measurements when combined with theoretical spectroscopic techniques.
As an illustration, we delve into recent micro-ARPES measurements of TMDs on top of black phosphorus. Band unfolding precisely captures the energy and angular dependence of mini-gaps appearing in the TMDs electronic band structure, revealing insights into the rehybridization between two lattices featuring hexagonal and rectangular symmetry [1].
The excitonic response of twisted WSe_2 measured by electron energy loss spectroscopy (EELS) is also explained by combining the band unfolding of the extended moiré structure with simulations of the optical response of the simplest nontwisted systems obtained by a GW+BSE approach [2].

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