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Unfolding the electronic bands of 2D heterostructures

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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 a 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.
Here we show how band unfolding can help in understading angle-resolved photoemission spectroscopy (ARPES) but also other spectroscopic measurements when combined with theoretical spectroscopic techniques. As an example, we discuss with this *ab initio* approach the appearance of mini-gaps in the electronic structure of various stacked 2D heterostructures. The excitonic response of twisted semiconducting bilayers 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.

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