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Band unfolding calculations compared with ARPES experiments: Examples of Ni1/3TiS2 and twisted-bilayer graphene

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Electronic band structure calculations based on the density-functional theory (DFT) collaborating with Angle-Resolved-Photo-Emission Spectroscopy (ARPES) measurements is a very powerful tool to investigate the electronic properties of condensed matters. However, we often face a big problem of the "band folding", when we use the supercell scheme. The folded and "dense"electronic bands in the supercell Brillouin zone are not similar to the experimentally obtained band structures by ARPES anymore, which makes it difficult to compare them directly. Recently band unfolding method was proposed and used for many systems. In our recent studies, we applied the band unfolding method to Ni1/3TiS2 and compared it with the state of the art ARPES measurement. We have found that our band unfolding calculations give excellent agreement with the experiments, exhibiting the usefulness and validity of the band unfolding method. We have also applied the method to twisted-bilayer graphene.

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