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DFT vs ARPES: Comparing DFT Approaches for TMDCs Band Structure

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Layered transition metal dichalcogenides (TMDCs) are among the two-dimensional (2D) materials family. They have been extensively studied due to their intriguing physical properties and potential for many applications, for optical, electronic and optoelectronic devices.
Conventional solid-state band theory with density functional theory (DFT) has achieved a high degree of success in predicting electronic properties of materials despite the simplicity of the independent-electron model. Our aim here is to provide a systematic assessment of the accuracy of theoretical methods to determine the bulk and monolayer electronic band structures of 2D metal dichalcogenides.
The electronic structures of materials derived from ab initio calculations are compared with angle-resolved photoemission spectroscopy (ARPES) data.

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