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Band-structure effects in vertical layered-material heterostructures GABRIEL CONSTANTINESCU, University of Cambridge, UK, NICHOLAS HINE, University of Warwick, UK — By stacking 2D materials one can fine-tune the electronic structure properties of the component layers. We employ high-accuracy linear-scaling DFT calculations to explore large-scale models of transition metal dichalcogenide (TMDC) and hBN/Phosphorene heterostructures. Band modifications upon stacking and rotation of different monolayers can be obtained by unfolding the supercell spectral function into the primitive cells, allowing direct comparison to experimental ARPES results. Changes in spectral weight and band-structure between the monolayers and heterostructured interfaces show how lattice mismatch (TMDC/TMDC) or spacer layers (Phosphorene/hBN/Phosphorene) allow the component monolayers to retain more independence in heterostructures than in homostacks. Moreover, one can envision using cavities in spacer layers in order to confine the radial extent of a vertical heterostructure, with potential applications in optoelectronics.

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