Thickness-dependent valence band evolution of exfoliated hBN from monolayer to bulk revealed by microARPES

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Hexagonal boron nitride (hBN) serves as the ubiquitous dielectric, encapsulation layer, and tunnelling barrier for graphene and van der Waals devices, yet a systematic experimental benchmark of its electronic band structure as a function of thickness remains missing[1-3]. Here we report a comprehensive micro-focused angle-resolved photoemission spectroscopy (microARPES) study of mechanically exfoliated hBN spanning monolayer, bilayer, trilayer, four-layer, thin flakes, and bulk flakes, measured under identical calibration and analysis protocols. By mapping the valence band dispersion across the Brillouin zone and extracting energy- and momentum-resolved line shapes, we track the evolution of the valence-band maxima, bandwidth, and spectral broadening with increasing layer number. The data reveal a clear crossover from a two-dimensional limit to a bulk-like regime, manifested by the progressive emergence of interlayer coupling induced band splitting and thickness-dependent renormalization of the valence band maximum. Quantitative trends of the valence band maximum energy and linewidths provide direct constraints for minimal tight-binding/density functional theory descriptions of multilayer hBN and enable a practical reference for band alignment in graphene/hBN heterostructures. Our findings establish an experimental thickness series for hBN that is immediately pertinent to the design and interpretation of graphene and two-dimensional material devices where the hBN thickness serves as a key control parameter.

References

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Figures

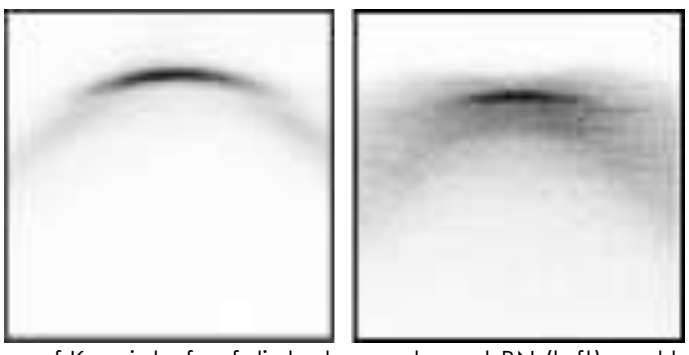

Figure 1: Electronic structure of K-point of exfoliated monolayer hBN (left) and bulk hBN (right).