Resonant interlayer coupling in $NbSe_2$-graphite epitaxial moiré superlattices

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Abstract

Moiré superlattices provide a powerful route to control the electronic structure of two-dimensional quantum materials through momentum-selective interlayer hybridization. Here, we study epitaxial $NbSe_2$/graphite, where lattice mismatch and aligned crystallographic axes generate a moiré potential linking electronic states of distinct character [1]. In our theoretical description, this potential acts as a resonant scattering channel, reconstructing bands when states in the two layers overlap in momentum and energy. As shown in Figure 1, *ab-initio* calculations combined with a real-space interlayer-coupling reproduce the angle-resolved photoemission spectra (ARPES) and capture the Umklapp scattering processes responsible for the band reconstruction. This is especially important in $NbSe_2$, where collective phases are highly sensitive to the band structure. The large lattice mismatch produces a large moiré wavevector, enabling graphite π states to hybridize with $NbSe_2$ states at the Fermi surface, where the charge-density-wave gap is maximal [2]. The moiré-induced hybridization therefore directly interferes with the underlying collective order. More broadly, these results identify resonant interlayer coupling as a mechanism by which epitaxial moiré superlattices reconstruct energy bands and tune ordered phases in two-dimensional quantum materials.

References

[1] Mak, K.F., Shan, J., Nature Nanotech. 17, 686–695 (2022)
[2] Xi, X., Zhao, L., Wang, Z. et al., Nature Nanotech. 10, 765–769 (2015).

Figures

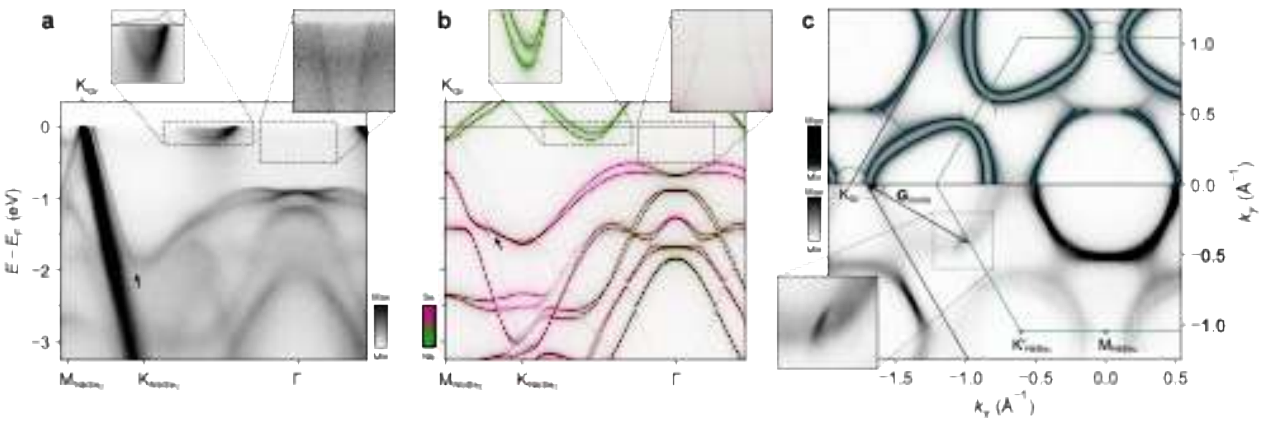

Figure 1: a) Measured ARPES dispersion of the $NbSe_2$/graphite heterostructure along the Γ-K-M direction. (b) Corresponding model calculations of the expected dispersion of the heterostructure. (c) Equivalent model calculations (top) and measurements of the Fermi surface.