Periodic Quasiparticle Energy Band Tunability in Striped MoS₂ Superstructures

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Abstract

Although the recently discovered monolayer transition metal dichalcogenides (TMDCs) exhibit novel electronic and optical properties, fundamental physical issues such as the quasiparticle band-gap tunability and substrate effects remain undefined. Herein, we present the first report of a quasi-one-dimensional periodically striped superstructure for monolayer MoS₂ on Au(100). The formation of the unique striped superstructure is found to be mainly modulated by the symmetry difference between MoS₂ and Au(100) and their lattice mismatch. More intriguingly, we find that the monolayer MoS₂ is heavily n-doped on the Au(100) facet with a bandgap of 1.3 eV; the Fermi level is upshifted by ~0.10 eV on the ridges (~0.2 eV below the conduction band) in contrast to the valley regions (~0.3 eV below the conduction band) for the striped patterns. This tunable doping effect is considered to be mediated by the weak/strong coupling effects between MoS₂ and Au(100) with respect to the ridge/valley regions. Additionally, an obvious bandgap reduction is observed in the vicinity of the domain for monolayer MoS₂ on Au(100). This work should therefore inspire intensive explorations of adlayer-substrate interactions and their effects on band-structure engineering of monolayer MoS₂.

References

- (1) Mak, K. F.; Lee, C.; Hone, J.; Shan, J.; Heinz, T. F. Phys. Rev. Lett. 105 (2010) 136805.
- (2) Song, C.-L.; Wang, Y.-L.; Cheng, P.; Jiang, Y.-P.; Li, W.; Zhang, T.; Li, Z.; He, K.; Wang, L.; Jia, J.-F.; *et al. Science* **332** (2011) 1410–1413.

Figures

