Growth and electronic structure of quasi-freestanding TMD heterostructures

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Abstract

Growth of two-dimensional (2D) materials under ultra-high vacuum (UHV) conditions allows for an in-situ characterization of samples with direct spectroscopic insight [1,2]. In order to preserve and study intrinsic properties, a preparation on substrate with minimal interaction is necessary. This can be realized by molecular beam epitaxy (MBE) on van der Waals (vdW) type substrates [3]. Heteroepitaxy of transition metal dichalcogenides (TMDs) in UHV remains a challenge for integration of several different monolayers into new functional systems. In this work we use two–step MBE to grow lateral and vertical TMD heterostructures on graphene as a combined 2D system. Size scalabillity of lateral-vertical heterostructure system of MoS_2 and WS_2, ranging from a quantum dot size to a semi-closed layer, is accomplished by coverage variation in subsequent preparations. We show that the growth method is invariant to a selection of TMD by preparing a similar heterostructure system with MoS_2 and TaS_2. Moreover, we demonstrate that three subsequent MBE preparations leads to novel quasi-freestanding heterostructure with MoS_2, TaS_2 and WS_2 segments as building blocks.
By means of scanning tunneling spectroscopy (STS), we examine the electronic structure of monolayer MoS_2, WS_2, and WS_2/MoS_2 vertical heterostructure. Moreover, we investigate a band bending in the vicinity of narrow one-dimensional (1D) interface of the WS_2-MoS_2 lateral heterostructure and mirror twin boundary (MTB) in the WS_2/MoS_2 vertical heterostructure. Density functional theory (DFT) is used for the band structure calculation, as well as for the density of states (DOS) maps characterization of the 1D interfaces. For the WS_2-MoS_2 lateral heterostructure we confirm type-II band alignment and determine corresponding depletion regions, charge densities and the electric field at the interface. For the MTB we observe a symmetric upward band bending and relate it to the dielectric screening of graphene acting dominantly on the MoS_2 layer. Quasi-freestanding heterostructures with sharp interfaces, large built-in electric field, and narrow depletion region widths are proper candidates for future designing of electronic and optoelectronic devices.

References

[1] C. Murray et al, *ACS Nano*, **14**, 7, 9176–9187, 2020
[2] Y. Dai et al, *ACS Appl. Mater. Interfaces*, **11**, 46, 43766–43773, 2019
[3] J. Hall et al, *2D Mater.* **5** 025005, 2018

Figures