Identification of PL emissions from Interlayer Excitons in 2D van der Waals Heterostructures

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1. Introduction

Two-dimensional (2D) semiconductors, including MoS_2, WS_2, $MoSe_2$, etc., have provided a fascinating opportunity to explore optical properties in 2 dimensions. In particular, van der Waals (vdW) heterostructures composed of these 2D semiconductors, such as WS_2/MoS_2, offer a novel platform for optical physics arising from interlayer excitons. It is, however, not straightforward to understand optical response from interlayer excitons because contributions from interlayer excitons with different transition energies overlap to a show broad peak in optical spectra. In this work, we have focused on the assignment of PL emission from interlayer excitons by using *h*BN-sandwiched high-quality samples.

2.Results and discussion

We synthesized monolayer MoS_2 and WS_2 by chemical vapor deposition method and prepared thin hBN flakes by mechanical exfoliation method. *h*BN-encapsulated heterostuructures (*h*BN/WS_2/MoS_2/*h*BN) were prepared with the polymer-assisted dry-transfer method. Figure 1 shows PL spectrum of a (*h*BN/WS_2/MoS_2/*h*BN) sample measured at room temperature under ambient condition. In addition to the A-exciton peaks around 1.8-2.0 eV, emissions, which is absent in PL spectra of monolayer WS_2 or MoS_2, can be seen at 1.4-1.7 eV. These PL peaks, which can be decomposed to three peaks, are observed only in heterostructure samples, being assigned to interlayer excitons. Through detailed PL measurements and comparison with calculated joint density of states, we have concluded that the three PL peaks originate from interlayer exctions corresponding to direct transition from K-point to K-point; indirect transition from K and Q-point to Gamma point. We think that these assignments were achieved due to the quality of our samples achieved by *h*BN encapsulation.

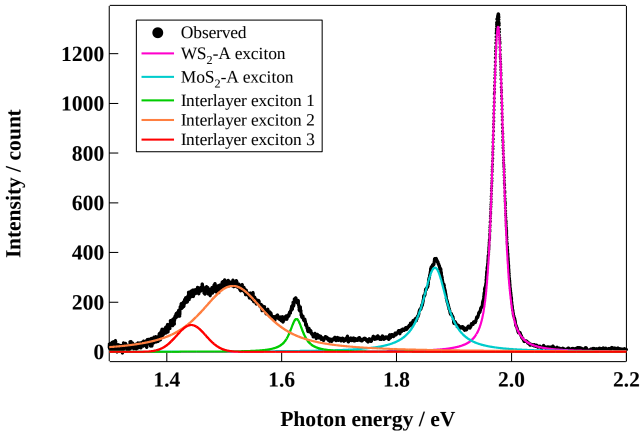

Fig.2 PL spectrum of *h*BN-encapsulated WS_2/MoS_2 vdW heterostructure.

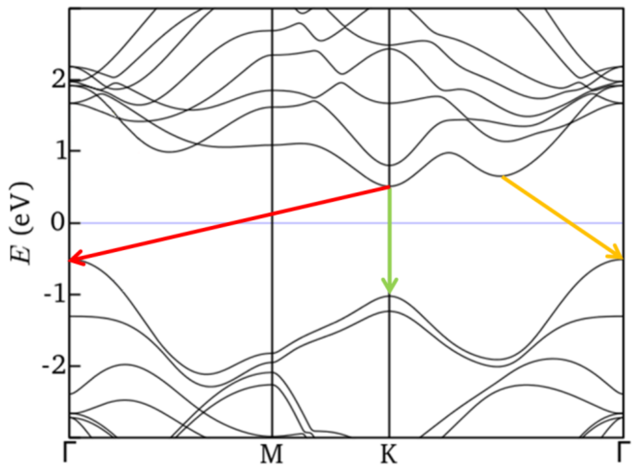

Fig.2 Band structure of WS_2/MoS_2 vdW heterostructure obtained by DFT calculation. Vectors correspond to transition of interlayer exciton shown in fig. 1.

3. Conclusions

We have successfully assigned PL emission from interlayer excitons of *h*BN-encapsulated WS_2/MoS_2 vdW heterostructure. Appearance of the sharp interlayer exciton peak clearly demonstrates that the quality of the fabricated is high. The results obtained in this work indicate the importance of hBN encapsulation in investigation of intrinsic physical properties of TMDC vdW heterostructures.

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