Supplementary Material

Different types of band alignment at MoS₂/(Al, Ga, In)N heterointerfaces

Deependra Kumar Singh,¹ Basanta Roul,^{1,2} Rohit Pant,¹ Arun Malla Chowdhury,¹ K. K. Nanda,^{1,a)}
and S. B. Krupanidhi^{1,b)}

1: Materials Research Centre, Indian Institute of Science, Bangalore – 560012, India

2: Central Research Laboratory, Bharat Electronics, Bangalore – 560013, India

a) nanda@iisc.ac.in

b) sbk@iisc.ac.in

The FWHM values of MoS₂/InN is the highest, followed by MoS₂/AlN, and the value for MoS₂/GaN is the least, thus indicating that growth quality of MoS₂ on GaN is best among the three (Fig. S1).

FIG. S1. Peak fitting of the two Raman modes of MoS₂ in different MoS₂/III-nitrides. The FWHM (w) values of the corresponding spectra have been shown along (marked by a red rectangle).

The AFM images of the top surface of MoS₂/(Al, Ga, In)N are shown in Fig. S2. It can be seen that the MoS₂ films are quite smooth, with some particulate formation in all the three samples. The root mean square (rms) surface roughness values for MoS₂/AlN, MoS₂/GaN, and MoS₂/InN are found to be 0.571, 0.501, and 1.26 nm, respectively.

FIG. S2. AFM scans of top surface of different MoS₂/III-nitrides. The RMS roughness (R_q) values of the corresponding surfaces have been shown along (marked by a red rectangle).

The band offsets for different MoS₂/III-nitrides determined by HRXPS measurements are shown in **Fig. S3**.

FIG. S3. For MoS₂/InN: (a) Mo3d core level and valence band spectra acquired from MoS₂, (b) In3d and Mo3d core level spectra of MoS₂/InN heterojunction, (c) In3d core level and valence band spectra of InN epilayer; for MoS₂/GaN: (d) Mo3d core level and valence band spectra acquired from MoS₂, (e) Ga2p and Mo3d core level spectra of MoS₂/GaN heterojunction, (f) Ga2p core level and valence band spectra of GaN epilayer; and for MoS₂/AlN: (g) Mo3d core level and valence band spectra acquired from MoS₂, (h) Al2p and Mo3d core level spectra of MoS₂/AlN heterojunction, (i) Al2p core level and valence band spectra of AlN epilayer. Peak positions are marked in the parentheses.

Figure S4 is a schematic of the comparison of band alignments of MoS₂ with different III-nitrides obtained from the above HRXPS results.

FIG. S4. Band alignment at (a) MoS₂/InN, (a) MoS₂/GaN, (c) MoS₂/AlN, and (d) schematic of band alignments of MoS₂ with the III-nitride semiconductors (All energy values are in eV).