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Abstract title: Impact of precursor chemistry on energy band alignment of few layer MoS2 grown by AP-CVD at interface with SiO2.

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Abstract

Recent advances in the fabrication of two-dimensional transition metal dichalcogenide (2D-TMD) semiconductors opened exciting possibilities in a wide range of applications in electronics, photonics, and optoelectronics. Especially, few layers molybdenum disulphide (MoS_2) have attracted tremendous interest as channel material for overcoming the short-channel effects in ultra-scaled field-effect transistors (FETs). Here we present the study of the energy band alignment at MoS_2/SiO_2 interface using internal photoemission (IPE) spectroscopy. A clear understanding of the energy alignment of electron bands is essential for the design of MoS_2 based devices. For example, in electrical measurements such as current, capacitance, etc, a high lateral resistivity in few layer semiconductor (or FL-MoS_2) films impairs lateral measurements. Therefore, here we employed IPE that is capable to characterize the energy band alignment also on discontinuous films through observation of electron transport in the direction normal to the interface.In this work, few layer MoS_2 films were grown on SiO_2(50nm)/Si using ambient pressure chemical vapor deposition (AP-CVD) from different metal precursors and with the use of different (i) organic (PTAS) and (ii) inorganic promoters, namely Na(OH), KCl and KI. The so-grown MoS_2 samples were analysed using IPE, to determine the electron energy position of the semiconductor valence band (VB) of MoS_2 relative to the reference level of the conduction band (CB) of SiO_2. (i) Firstly, using IPE spectroscopy, Powell’s plots of IPE quantum yield spectra for CVD grown 6L-MoS_2 from PTAS seed promoter were built with optically semi-transparent Au contacts for gate biases ranging between -2 and -9 V. A linear extrapolation to the zero electric field yields the high-energy threshold $\Phi_{MoS2} = 4.2 \pm 0.1$ eV for PTAS assisted MoS_2. In bare 6L-MoS_2 a lower IPE threshold $\Phi_{MoS2} = 3.7 \pm 0.1$ eV energy was reported. Interestingly, a significant (≈ 500 meV) barrier enhancement is found in the case of PTAS compared to the case without PTAS. This observation points towards a possible effect of a dipole layer or doping, induced by PTAS. (ii) In the case of inorganic promoters, we observed the MoS_2 VB position in the range $\Phi_{MoS2} = 3.6$ to 4.2 ± 0.1 eV with an estimated difference of ≈300 meV if using different precursor chemistry during the MoS_2 growth. This VB shift is tentatively ascribed to the formation of an interface dipole due to inorganic seed residuals (such as OH, Cl) attached to SiO_2 interface. In addition, we discuss perspectives on the implementation of seed promoter assisted MoS_2 AP-CVD growth.