Evidence for Highly p-type doping and type II band alignment in large scale monolayer WSe_2 /Se-terminated GaAs heterojunction grown by Molecular beam epitaxy

Debora Pierucci[1], Aymen Mahmoudi[1], Mathieu Silly[2], Federico Bisti[3], Fabrice Oehler[1], Gilles Patriarche[1] Frédéric Bonell[4], Alain Marty[4], Céline Vergnaud[4], Matthieu Jamet[4], Hervé Boukari[5], Marco Pala[1], and Abdelkarim Ouerghi[1]

[1] Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies, 91120, Palaiseau, [2]Synchrotron-SOLEIL, Université Paris-Saclay, Saint-Aubin, BP48, F91192 Gif sur Yvette, France
[3]Dipartimento di Scienze Fisiche e Chimiche, Università dell'Aquila, Via Vetoio 10, 67100 L'Aquila, Italy
[4]Université Grenoble Alpes, CEA, CNRS, Grenoble INP, IRIG-Spintec, 38054, Grenoble, France
[5] Université Grenoble Alpes, CNRS and Grenoble INP, Institut Néel, F-38000 Grenoble, France

Azimuthal XRD scans at Bragg positions:

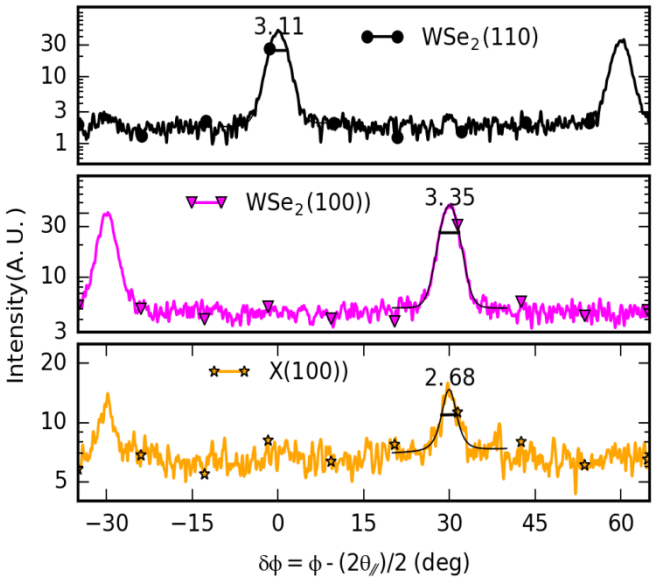

Figure S1: In-plane azimuthal XRD scans done with detector positioned at the Bragg angle of WSe_2(110), WSe_2(100) and X(110) Bragg angles. The peaks are annotated with their full width at half maximum which give the orientation distribution spread of the crystallites.

Energy Distribution Curves (EDC) analysis: The band positions were determined by energy distribution curve analysis (EDC) of the ARPES spectra as reported in Figures S2-S4. The fit was performed using a Shirley background (arctangent function as background) and a Gaussian (Lorentzian) line shape for the peaks in the case of K points of WSe_2 on Se-terminated GaAs (Graphene), and for the Γ point of Se-terminated GaAs.

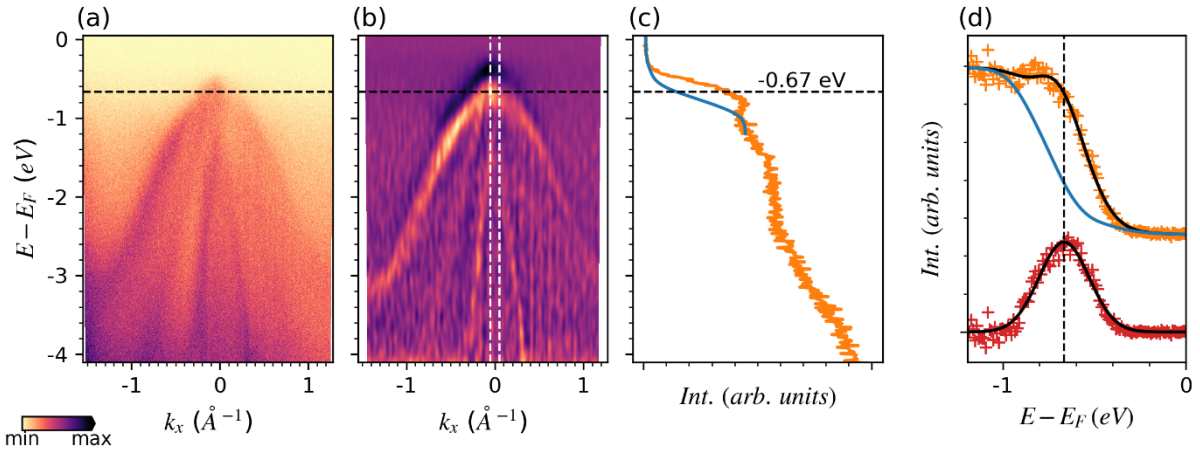

Figure S2: Energy position determination for the lowest bonded GaAs band at Γ. (a) the ARPES spectra of WSe_2/Se-terminated GaAs probed with 120 eV photon energy; (b) the filtered ARPES spectra using a Laplacian of Gaussian filter; white dashed line indicates the region of integration for the EDC; (c) the EDC signal (in orange) with the Shirley background (blue line); (d) the EDC signal (in orange), the Shirley background (blue line), the background subtracted EDC signal (in red), the fitted line shape (black lines). Dashed black lines in all the panels indicate the energy of the peak position.

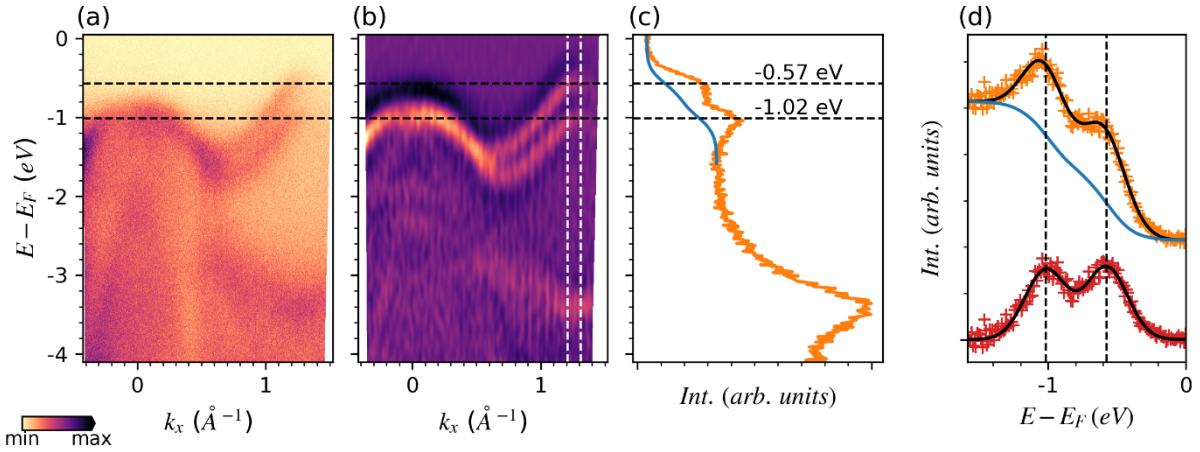

Figure S3: Energy position determination for the two lowest bonded WSe_2 band at K. (a) the ARPES spectra of WSe_2/ Se-terminated GaAs probed with 60 eV photon energy; (b) the filtered ARPES spectra using a Laplacian of Gaussian filter; white dashed line indicates the region of integration for the EDC; (c) the EDC signal (in orange) with the Shirley background (blue line); (d) the EDC signal (in orange), the Shirley background (blue line), the background subtracted EDC signal (in red), the fitted line shape (black lines). Dashed black lines in all the panels indicate the energy of the peak position.

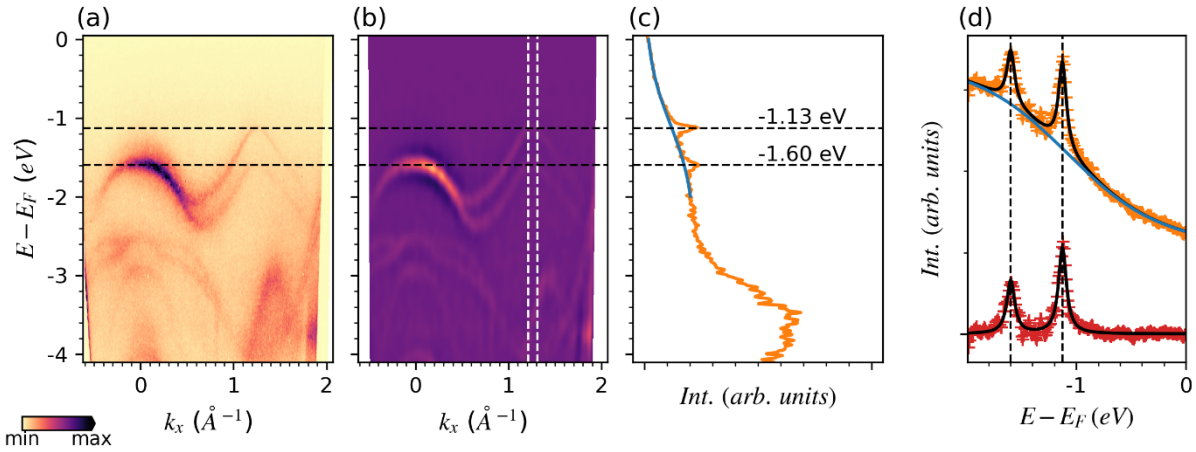

Figure S4: Energy position determination for the two lowest bonded WSe_2 band at K. (a) the ARPES spectra of WSe_2/graphene; (b) the filtered ARPES spectra using a Laplacian of Gaussian filter; white dashed line indicates the region of integration for the EDC; (c) the EDC signal (in orange) with the arctangent function as background (blue line); (d) the EDC signal (in orange), the arctangent function as background (blue line), the background subtracted EDC signal (in red), the fitted line shape (black lines). Dashed black lines in all the panels indicate the energy of the peak position.

Work Function measurements: The work function (WF) of the sample was determined by the measurement of the secondary electron (SE) edge with a photon energy of 120 eV. In order to ensure that the SE has a kinetic energy (KE) higher than the analyser vacuum level, the sample is negatively biased (-18 V) with respect to the analyser. The secondary electron energy distribution curve is shown in Figure S5 as a function of the kinetic energy referenced at the Fermi level. Consequenly, the secondary electron cut-off (KE_{cutoff}), measured by extrapolating the edge of the peak to the zero baseline (Figure S5) gives directly the value of the workfunction, which is found to be 4.90 ± 0.05 eV.

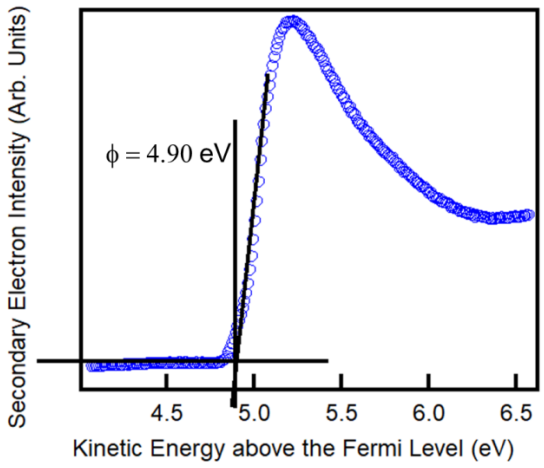

Figure S5: Secondary electron intensity as a function of the kinetic energy above the Fermi level for the WSe_2/ Se-terminated GaAs heterostructure measured with hν = 120 eV.