Evolution of Band Structure in 2D Transition Metal Dichalcogenide Alloy $Mo_xW_{1-x}Se_2$

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Abstract. Among the plenty of two-dimensional (2D) materials emerged in the research scenario after the discovery of graphene, transition metal dichalcogenides (TMDCs) attract huge interest as potential functional material candidate for electronic and optoelectronic applications. Various TMDCs with the general formula MX_2 (M=Mo, W; X=S, Se, Te) usually exhibit a distinct bandgap and spin polarized bands. There are many artificial methods put forward to engineer the bandgap and spin polarized bands such as chemical doping, induction of strain or external electric field etc. Recent developments in the synthesis of TMDCs open up a new family of materials called 2D TMDC alloys [1]. Here we are studying the band structure of $Mo_xW_{1-x}Se_2$ single crystals with various stoichiometric ratio x in comparison with WSe_2. The structural characterisation of samples was analysed using Low energy electron diffraction [LEED] and Scanning Electron Microscopy (SEM) with Energy Dispersive X-Ray Analysis (EDX). The core level spectra of the samples were obtained using X-ray photoemission spectroscopy (XPS). Angle Resolved Photoemission Spectroscopy (ARPES) was used to investigate the electronic band structure of the samples. We evaluated the band dispersion and also observed the splitting of the bands at the K point [2]. We compare the ARPES results with one step model photoemission calculations using SPR-KKR [3] to explain if the origin of these changes are due to chemical or matrix elements effects. Thus we are evaluating the potential way for band engineering of the TMDC family.

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