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The observation of strain-induced valence band splitting on $HfSe_2$ by Alkali metal intercalation

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Alkali metal intercalation in layered-transition metal dichalcogenides (LTMDs) has been intensively studied due to a wide range of attractive properties such as enhancement of superconductivity, quasi-freestanding, and negative electron compressibility which lead to many potential nanoelectronic applications. Essentially, many researchers study the correlation between electron doping and strain (and vice versa) in order to manipulate their electronic structure, band gap, and carrier mobility. In this work, we have measured the electronic structure of 1T-$HfSe_2$ by using angle resolved photoemission spectroscopy (ARPES) together with $in\ situ$ alkali metal evaporation. Our ARPES data as a function of electron doping show the monotonic increase of in-plane p-orbital valence band splitting (VBS) reaching as high as 350 meV and the band gap reduction up to 250 meV for a carrier density around 5x10^{14} cm^{-2} (corresponding to ˜20% of Brillouin zone). These VBS values are very similar over various alkali metal dopants (including Na, Cs, and Rb) suggesting that the in-plane lattice reduction is dominated while the out-of-plane lattice expansion is neglected at the valence band maximum. The density functional theory calculation (DFT) has been used to understand the electronic structure of $HfSe_2$ under the condition of alkali metal intercalation and strain. At 25% of Na doping, the out-of-plane lattice constant (c) increases up to 11% while the in-plane lattice constant (a) decreases around 3% which can be described by the different coulomb interaction over Se atoms. The calculation of electronic structure under uniaxial tensile strain is very well in agreement of our ARPES data in both of VBS and band gap shrinkage indicating that uniaxial strain can be induced by alkali metal intercalation. Finally, our finding should help to simplify the study in strain physics as well as for large-scale strain engineered devices.

Keyword: alkali metal intercalation, layered-transition metal dichalcogenides, strain, angle resolved photoemission spectroscopy, density functional theory.

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