Oxygen Induced Intra- and Inter-layers Modification of β-InSe: Formation of Pseudo-heterojunction

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Easy band gap control of InSe is a necessary feature for next generation 2D materials. InSe is attracting considerable attention due to its promising electrical and optoelectronic properties although it is vulnerable to oxidation. However, the variety of oxidation of InSe has not yet been clearly understood [1, 2]. Here, we unveil the missing early step of oxygen adsorption resulting in alternation of intra- and inter-layer properties by using *in-situ* soft X-ray spectroscopy for three different oxidation conditions. Se vacancies or $InSe_x$ provides energetically favorable sites of which oxidation reproduces vacancy defects. At room temperature, the reactivity of Se is observed to be greater than that of In. However, annealing or surface etching induces In oxidation. In the early stages, chemisorption is not energetically favored, and instead the physically adsorbed oxygen increases the hole density without changing the electronic structure of the valence band, resulting in p-doping. Further exposure to oxygen initiates chemical transformation, resulting in the formation of SeO_2. The chemically modified surface layers are electron-rich and generate a photovoltaic response. This study deepens our understanding of surface oxidation of InSe, which appeared in different way depending on environments.

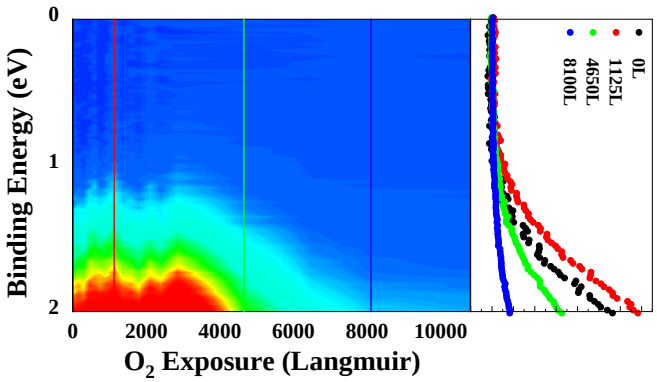

Fig. 1 Electrical property change of InSe according to oxidation progress. Scheme of the valence band structure base on the Fermi level (E_F, 0eV) as a contour map

[1] P.-H. Ho *et al.*, (s), ACS Nano, **11**, 7362 (2017)
[2] H. Nan *et al.*, Semiconductor Science Technology, **33**, 074002 (2018)