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Carrier Transport and Origins of Narrow Bandgap for P-type Layered Semiconductor, β-$BaZn_2As_2$

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Background and Objective: $BaZn_2As_2$ is a layered crystal composed of alternating stacking of a Ba layer and a ZnAs layer, and takes an orthorhombic lattice at the standard condition. It is expected for a good *p*-type semiconductor because largely-spread As 4*p* orbitals would form highly-dispersed valence band maximum. Here, we report epitaxial growth of a tetragonal β-$BaZn_2As_2$ phase and discuss its electrical properties and electronic structure.

Experimental: Epitaxial $BaZn_2As_2$ films were grown on single-crystal MgO (001) substrates by a reactive solid-phase epitaxy technique. Structural, optical and electrical properties were measured at room temperature. Valence band spectra were measured by hard X-ray photoemission spectroscopy (HAX-PES) at BL15XU beamline of SPring-8. Density functional theory calculations were performed with the hybrid HSE functionals using a code VASP 5.3.3.

Results and Discussion: X-ray diffraction confirmed that the grown films were tetragonal β-$BaZn_2As_2$ grown epitaxially on the MgO (001), and the films exhibited *p*-type conduction with high conductivity of ~0.1 S/cm. However, optical absorption spectra showed that its bandgap is as small as ~0.2 eV, which is unexpectedly smaller than that of a family compound LaZnOAs (1.5 eV). To clarify its origin, we performed HSE calculations, which gave a good explanation of its bandgap (0.22 eV) and reproduced the experimental valence band spectra (Fig. 1). At the conference, we will discuss the origin of its narrow bandgap.

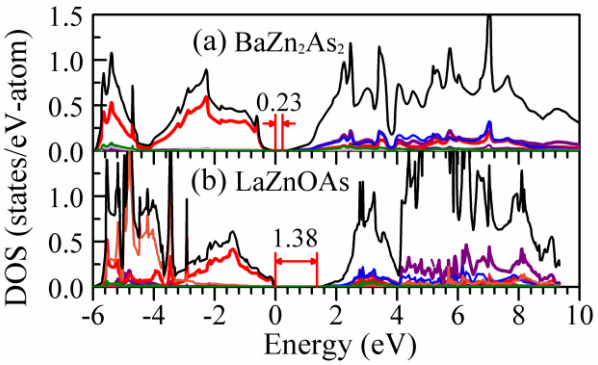

Fig. 1. PDOSs of (a) $BaZn_2As_2$ and (b) LaZnOAs calculated with HSE hybrid functional.