Electronic structures of Zn-Pn (Pn = P, As, Sb)-based layered crystals

Xiao Zewen\textsuperscript{a}, Toshio Kamiya\textsuperscript{a}, Hidenori Hiramatsu\textsuperscript{a} and Hideo Hosono\textsuperscript{a,b}

\textsuperscript{a} Tokyo Institute of Technology, Tokyo 226-8503, Japan

zwxiao@lucid.msl.titech.ac.jp

Although n-type oxide semiconductors exhibit large electron mobilities \( \sim 200 \text{ cm}^2/(\text{Vs}) \) for single crystals and \( > 10 \text{ cm}^2/(\text{Vs}) \) even for amorphous oxides. On the other hand, it is much difficult to find a high-mobility p-type oxide in particular in an amorphous phase. We have reported that SnO and Cu\(_2\)O can produce p-channel thin-film transistors (TFTs), and SnO TFTs now exhibit several \( \text{cm}^2/(\text{Vs}) \) of field-effect mobilities. Although we have also reported other p-type materials such as LaCuChO (\( Ch = S, \text{ Se, Te} \)), Cu\(_2\)Ch, but their TFTs did not work. For related compounds, we have synthesized bulk samples and grown thin films for LaZn\(_n\)PnO (\( Pn = P, \text{ As, Sb} \)), but their resistivity were high and carrier polarity was not determined clearly. In addition, LaZn\(_n\)PnO has a complex chemical composition and contains high-melting point element, La; therefore, it requires a high temperature to grow high-quality films. On the other hand, from the knowledge of iron-pnictide superconductors, it is known that 122-type compounds like BaFe\(_2\)As\(_2\) are more easy to grow epitaxial films than 1111-type compounds like LaFeAsO. In this work, we focus on 122-type compounds BaZn\(_2\)Pn\(_2\) and related compounds and compare their electronic structures.

LaZn\(_n\)PnO and BaZn\(_2\)Pn\(_2\) are composed of common Zn\(_n\)Pn layers and the Zn\(_n\)Pn layers contribute to carrier conduction and form the bandgap. However, density functional theory (DFT) calculations using VASP 5.3 indicated that the bandgaps of LaZn\(_n\)PnO are larger than those of corresponding BaZn\(_2\)Pn\(_2\), and the DFT bandgaps of BaZn\(_2\)Pn\(_2\) become even negative. To correct the DFT bandgap problem, we examined different hybrid functionals and found HSE would provide a good explanation for experimental results. It indicates that the band gap of LaZnPO is 1.51 eV, while that of BaZn\(_2\)P\(_2\) is 0.42 eV. We will discuss them in comparison with experimental bandgaps at the conference.