First-principles study of the effect of uniaxial pressure on α-$SnWO_4$

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Tin tungstate ($SnWO_4$) crystallizes below 670°C in orthorhombic α-phase (Fig. 1(a)) [1] with narrow band gap (E_g=1.7 eV [2]). For use as transparent semiconductor, it can be produced in thin-film form by magnetron sputtering method [2]. It was shown recently [3,4] that external hydrostatic pressure can induce in α-$SnWO_4$ a transition into conducting state. The influence of stress is anticipated in tungstate nanostructures and thin films.

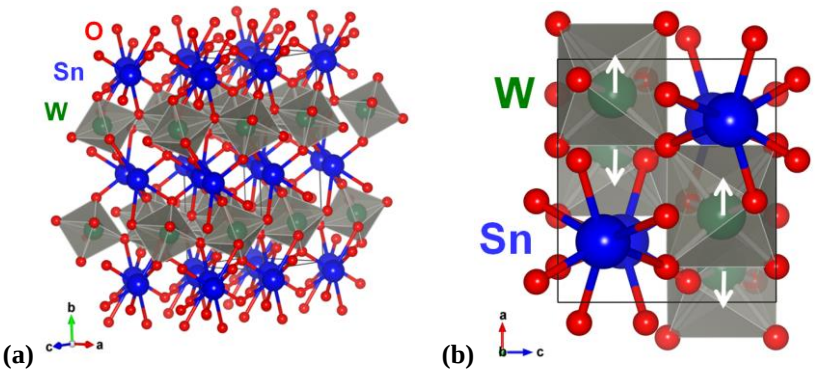

Fig. 1. (a) Crystalline structure of α-$SnWO_4$. (b) A fragment of α-$SnWO_4$ structure in the *ac*-plane. Arrows indicate the displacement directions of tungsten atoms under uniaxial pressure along *a*- or *c*-axis.

In this study the effect of uniaxial pressure on the atomic and electronic structure of α-$SnWO_4$ was investigated by means of first-principles linear combination of atomic orbital (LCAO) method employing density functional theory (DFT)/Hartree-Fock (HF) hybrid functional. It was found that uniaxial stress affects a degree of WO_6 and SnO_6 octahedra distortion, caused originally by the second-order Jahn-Teller effect (Fig. 1(b)). Moreover, a compression along *a*- or *c*-axis leads to a collapse of the band gap, whereas the gap increases upon a compression along *b*-axis.

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References

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