Crystal Structure and Optoelectronic Properties of Hexagonal M*x*WO_3

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Hexagonal tungsten bronze (HTB) M*x*WO_3 (M= alkali metal; $0.19 \leq x \leq 0.37$) has been studied in recent years because it has the excellent shielding characteristic in the range of near infrared (NIR) and ultraviolet wavelengths. It can be used as thermal insulation layer in the field of architectural and automotive window glasses. To improve the NIR-shielding performance HTB, it is imperative to confirm the crystal structure and then make clear the NIR-shielding mechanism of $Cs_{0.33}WO_3$ for enhancing the NIR-shielding efficiency.

To produce single crystal via molten-salt method. The crystal structure was also analyzed and refined with a full-matrix least-squares method of the Bruker SHELTAL software package based on the XRD intensity data. Consequently, the experimental results indicate that the space group of the HTB is $P6_322$.

The absorption spectra of Cs*x*WO_3 nanoparticles clearly exhibit that the absorption with the maximum transmission percent of visible light occurred at wavelengths close to 530 nm and NIR were cut off in the range of 900 to 2100 nm.

In order to quantitatively describe the electronic and bonding behavior of the $M_{0.33}WO_3$, the *ab* initio structure relaxations were performed using Density Function Theory within the Local Density Approximation, as implemented in the VASP code.