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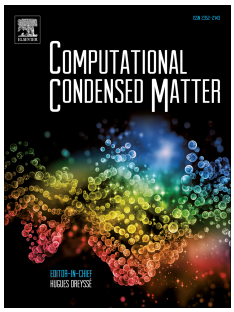


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# Effect of pressure on the structure stability, electronic structure and band gap engineering in $Zn_{16}O_1S_{15}$

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## Abstract

Crystal structures and high pressure structural phase transitions of $Zn_{16}O_1S_{15}$ have been investigated using density functional theory calculation. The two candidate high pressure structures namely Wurtzite and Zincblende were examined for theirs stability and properties up to 20 GPa. The co-exist phase of both structure which occurred during the difference film growth conditions was fully explained. Phonon dispersion and the Born criteria reveal that Zincblende is only stable up to 10 GPa. Besides, Wurtzite structure yield no imaginary phonon frequencies and also satisfy the elastic constants sufficiency condition up to 20 GPa which indicated that the co-exist phase would eventually become the single Wurtzite structure above 10 GPa. The electronic structure and PDOS were also fully investigated using HSE06. The multiple band gap energy and mid O-3 state between fundamental ZnS band gap was revealed for the first time. The pressure effect on their electronic structure has been investigated for possible applications in adjustable optoelectronic device.

**Keyword**: II-VI ternary alloys, ab-initio calculation, Phase Stability, High Pressure, Density Functional Theory