

Abstract Submitted  
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**Exploration of the electronic structure properties of new tetrahedral oxides: zincites**<sup>1</sup> GIANCARLO TRIMARCHI, ARTHUR J. FREEMAN, Northwestern U., LINHUI YE, Peking University — The long standing chemical rules of isovalent species co-substitution allow, starting from adamantine semiconductors such as ZnS, to derive compounds such as the chalcopyrite-type CuGaS<sub>2</sub> in the same structural aristotype. These co-substitution rules when applied to tetrahedral oxides like ZnO, point to a field of compounds with underlying tetrahedral coordination, that is largely unsurveyed yet very promising for identifying new materials suited as transparent conducting oxides and perhaps photovoltaic adsorbers. We focus here on one such compound, derived from ZnO by a 3:1 co-substitution of Zn with Ag and V, Ag<sub>3</sub>VO<sub>4</sub>, as a paradigmatic component of this new compound field. The FLAPW method within the screened-exchange LDA scheme is employed to assess the band gap values, otherwise underestimated in simple LDA. The two main polymorphs of Ag<sub>3</sub>VO<sub>4</sub> are considered here, i.e.,  $\alpha$ - and  $\beta$ -Ag<sub>3</sub>VO<sub>4</sub>, both *daughter* structures of the *parent* adamantine lattice. Both forms show Ag and V d-like valence and conduction band edges, respectively, with a band gap that depends on the coordination of the Ag site and is close to the visible range. Our investigation suggests Ag<sub>3</sub>VO<sub>4</sub> to be a candidate co-substitution dopant of ZnO.

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