Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Influence of local environment on the characterization of the p-type TCO in silver vanadates[1] JINO IM, GIANCARLO TRIMARCHI, HAOWEI PENG, KENNETH POEPPELMEIER, ARTHUR FREEMAN, Northwestern University, Evanston, IL 60208, USA — Cu and Ag oxides are often considered as possible candidates for p-type transparent conducting oxides (TCO's) because the d^{10} valence structure usually gives rise to dispersive d-bands at the valence band maximum. Among them, multi-cation oxides of silver and vanadium show various atomic structures such as the $\alpha-$ and the $\beta-$phase of Ag_3VO_4 and $KAg_{11}(VO_4)_4$. Hence, these compounds, especially $KAg_{11}(VO_4)_4$, offer several local environments at Ag sites and it is interesting to assess how they influence the electronic structure. Based on first-principles density functional theory, we point out a relation between the local environment and d-s orbital mixing at the Ag site. In turn, this mixing determines the orbital composition of the band extrema and band gaps. The influence on band gaps of the substitution of Nb and Ta for V in Ag_3VO_4 and of the substitution of alkali metals for K in $KAg_{11}(VO_4)_4$ will also be discussed.

[1]Supported by the DOE EFRC for Inverse Design (Grant No. DE-AC36-08GO28308).

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Date submitted: 22 Dec 2010 Electronic form version 1.4