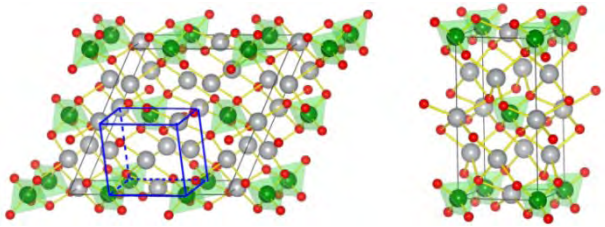
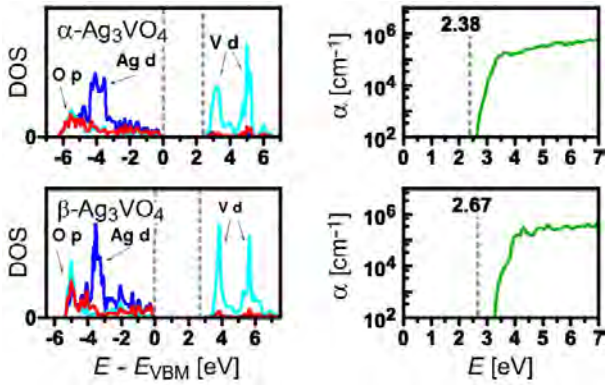
Ag_3VO_4 as a New *p*-Type Transparent Conducting Material

Using systematic design principles, the Center for Inverse Design is exploring a new class of ternary* p*-type transparent conducting oxides (TCOs), including the prototypical Ag_3VO_4 entry-point material.

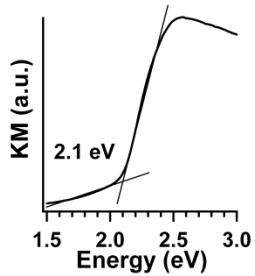
The simultaneous occurrence of transparency and *p*-type (hole-carrier) conductivity is an elusive materials property that could have high impact on technologies such as photovoltaics and transparent electronics. However, no satisfactory *p*-type TCOs are known to date. Therefore, our Center is using the inverse-design methodology to create new *p*-type TCOs. As an entry point, we considered the ternary $(Cu/Ag)_3VO_4$ compounds and theoretically predicted that hole producers (Cu/Ag-vacancies) will dominate hole killers (Cu/Ag interstitials, O vacancies). We synthesized Cu_3VO_4 and Ag_3VO_4 crystals with a novel hydrothermal technique. The prediction of extremely low formation energies of Cu-vacancies is validated by observing highly off-stoichiometric $Cu_{3-x}VO_4$ (x = 0.15); however, this compound is opaque according to both theory (E_g = 1.0 eV) and experiment. Ag_3VO_4 exists in two polymorphs—α- and β-Ag_3VO_4, with the α-form stable below 365 K—and both are predicted to be indirect semiconductors. The absorption edge of α-Ag_3VO_4 crystals at 2.1 eV (predicted indirect gap: 2.38 eV) is smaller than the 3.0 eV needed for transparency and the predicted intrinsic hole density up to ~10^{18} cm^{-3} stays below desired p-type doping levels. However, this research on Ag_3VO_4 lays the foundation for improved ternary *p*-type TCOs.



Crystal structure of α- (*left*) and β- (*right*) Ag_3VO_4



(Above) Theory: Density of states (DOS) and optical absorption profiles for Ag_3VO_4. *(Right)* Experiment: Diffuse reflectance of α-Ag_3VO_4.



Reference: G. Trimarchi, H. Peng, J. Im, A. Freeman, V. Cloet, A. Raw, K. Poeppelmeier, K. Biswas, S. Lany, and A. Zunger, *Phys. Rev. B* **84**, 165116 (2011).