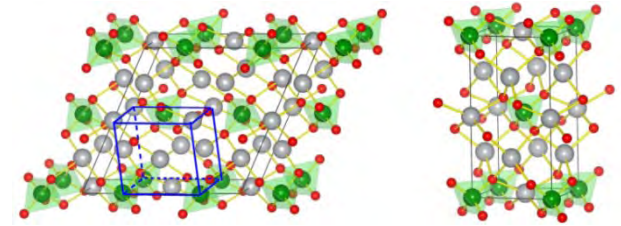


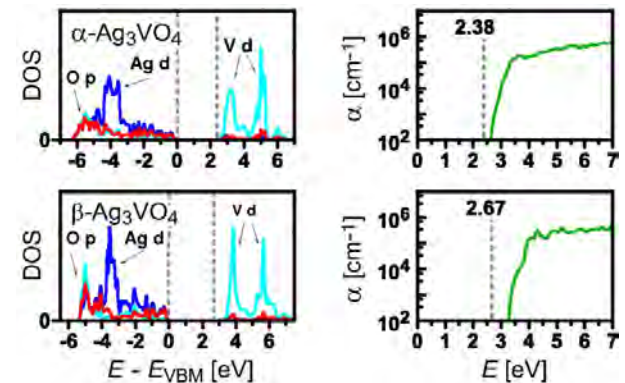
Ag₃VO₄ as a New *p*-Type Transparent Conducting Material

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 Ag₃VO₄ entry-point material.

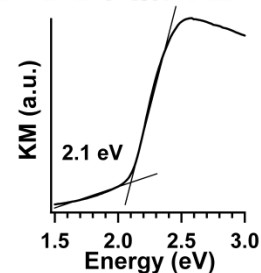
The simultaneous occurrence of transparency and *p*-type (hole-carrier) conductivity is an elusive materials property that could have high impact on technologies such as photovoltaics and transparent electronics. However, no satisfactory *p*-type TCOs are known to date. Therefore, our Center is using the inverse-design methodology to create new *p*-type TCOs. As an entry point, we considered the ternary (Cu/Ag)₃VO₄ compounds and theoretically predicted that hole producers (Cu/Ag-vacancies) will dominate hole killers (Cu/Ag interstitials, O vacancies). We synthesized Cu₃VO₄ and Ag₃VO₄ 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}VO₄ (*x* = 0.15); however, this compound is opaque according to both theory (*E_g* = 1.0 eV) and experiment. Ag₃VO₄ exists in two polymorphs—*α*- and *β*-Ag₃VO₄, with the *α*-form stable below 365 K—and both are predicted to be indirect semiconductors. The absorption edge of *α*-Ag₃VO₄ 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 ~10¹⁸ cm⁻³ stays below desired *p*-type doping levels. However, this research on Ag₃VO₄ lays the foundation for improved ternary *p*-type TCOs.



Crystal structure of *α*- (left) and *β*- (right) Ag₃VO₄



(Above) Theory: Density of states (DOS) and optical absorption profiles for Ag₃VO₄.
(Right) Experiment: Diffuse reflectance of *α*-Ag₃VO₄.



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).