

Abstract Submitted  
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**A database survey to search for new candidate *p*-type TCOs<sup>1</sup>** GIANCARLO TRIMARCHI, K. POEPPELMEIER, A. J. FREEMAN, Northwestern U., Evanston, IL — New *p*-type TCOs are often produced by reacting the prototype binary *p*-type oxides, i.e., Ag<sub>2</sub>O and Cu<sub>2</sub>O, with binary oxides of other transition metals or main-series elements. Yet, so far only a small part of all the multi-cation Cu and, in particular, Ag oxides have been assessed as candidate *p*-type TCOs. Furthermore, numerous multi-species Cu and Ag oxide systems are poorly characterized, which leaves ample scope for discovery of yet unknown compounds belonging to them, and, likely, of unsuspected new TCOs, too. Here, we survey a *complete* database of known multicomponent Ag and Cu oxides, without restrictions on element composition, to search for new candidate TCOs. We indexed all the compounds in this database by applying selected crystal structure descriptors as structure type, stoichiometry, and coordination environment of the Cu and Ag cations. Chemical insight points to a significant likelihood that 2- and 4-fold coordination of the noble metal cations yield band structure properties suitable for the transparency and hole conductivity needed in TCOs. We scanned the indexed database to find compounds that could match these requirements and identified a set of materials that could be interesting candidate *p*-type TCOs.

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