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Theoretical study of LaOXS {X=Cu, Ag} layered oxide sulphides[1] KANBER LAM, GIANCARLO TRIMARCHI, ARTHUR J. FREEMAN, Northwestern University — The ternary oxides, owing to the mismatch between the energy levels of the transition metal *d*-orbitals and the deep oxygen *p*-orbitals, typically show a limited dispersivity of the valence band maxima (VBM) and relatively heavy masses that make them not favorable in applications as p-type transparent conducting oxides (TCOs). In a hope to increase the *p*-*d* hybridization and preserve large band gaps in oxides with the addition of sulphur atoms, we studied the reported layered quarternary oxysulphides (LaCuOS, LaAgOS) using density functional theory with G0W0 self energy corrections. We confirmed that the VBM is mainly contributed by the antibonding state of Cu/Ag-*d* and S-*p* and the hole effective mass increases upon Cu substitution by Ag, which has a deeper *d* level than the Cu *d* one.

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