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First principles study of transition metal (TM=Pb, Cu) oxides/sulfides SEAN CAUDLE, MENG TAO, XIHONG PENG, Arizona State University — Earth-abundant transition meal oxides/sulfides have inspired special research attention recently due to their potential applications in solar cells. A clear understanding of the fundamental properties of these materials, especially the electronic properties and their tunability via chemical doping, are critically important towards the applications. In this presentation, we report first principles density-functional theory (DFT) study on the electronic structures of Pb and Cu oxides/sulfides and their oxysulfides compositions. The band structure and bandgap can be systematically tuned by increasing S component in the metal oxides. For example, the DFT predicted bandgap for PbO is 1.72 eV. While the bandgaps for $PbO_{0.937}$ $S_{0.063}$, $PbO_{0.875}S_{0.125}$, and $PbO_{0.75}S_{0.25}$ are 1.64 eV, 1.43 eV, and 0.79 eV, respectively. For Cu2O, the standard DFT seriously underestimates the bandgap to be 0.49 eV, compared to the experimental value of 2.17 eV. Two methods, DFT+U and hybrid functional (HSE06), were implemented to overcome this problem. Our results showed that DFT+U method fails and the bandgap doesn't further open up by providing a U potential. The hybrid functional predicts the bandgap to be 2.00 eV, which is in a good agreement with the experimental value.

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