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**Study of the Electronic Properties of Different Phases of Cu3V-VI4 Based on First-Principle Calculation** TINGTING SHI, WANJIAN YIN, The University of Toledo, MOWAFAK AL-JASSIM, National Renewable Energy Laboratory, YANFA YAN, The University of Toledo, YAN RESEARCH GROUP TEAM, THE MEASUREMENTS AND CHARACTERIZATION (M&C) GROUP COLLABORATION — Considering the small energy differences among the Cu3V-VI4 compounds in four different structures, enargite, wurtzite-PMCA, famatinite and zinc-blend-PMCA, a large variety of phases with different band properties may co-exist. This paper systematically studies the trend of the electronic properties of these phases; the band gap will greatly decrease when the phase changes from enargite to wurtzite-PMCA, or from famatinite to zinc-blende-PMCA. For example, the band gap of enargite Cu3PS4 is 2.51 eV, while the famatinite one is 1.72 eV. In addition, the band gap will obviously decrease as we increase the atomic number of group-V or group-VI element for one structure. Due to the wide band range from 0.4 eV to 2.5 eV for all possible Cu3V-VI4 structures, our detailed first-principle study will suggest guidelines for the band gap engineering for potential photovoltaic applications.

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