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Engineering of Bulk and Nano Materials for Energy Applications

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Materials design using first-principles techniques is one the ultimate goals in computational materials science. Due to the recent advancement in first-principles electronic structure theory and computing power, it is now possible to perform *knowledge-based* computational design of materials with unique optical, electrical, or magnetic properties that are tuned to specific energy related applications. This vital tool, therefore, has the great potential to accelerate scientific discovery of energy materials. In this talk, selective recent works from my group will be discussed to illustrate how computational methods can be used to design functional materials. Some of the examples include design of (i) solar cell absorber materials through cation mutation [1-3], (ii) bipolarly dopable transparent conducting oxides (TCO) for optoelectronic devices [4-8], (iii) filled tetrahedron alloys for solid state lighting applications [9-10], (iv) low band gap oxides for photoelectrochemical hydrogen production through water splitting [11-12], and (v) nano materials for energy storage [13-15].

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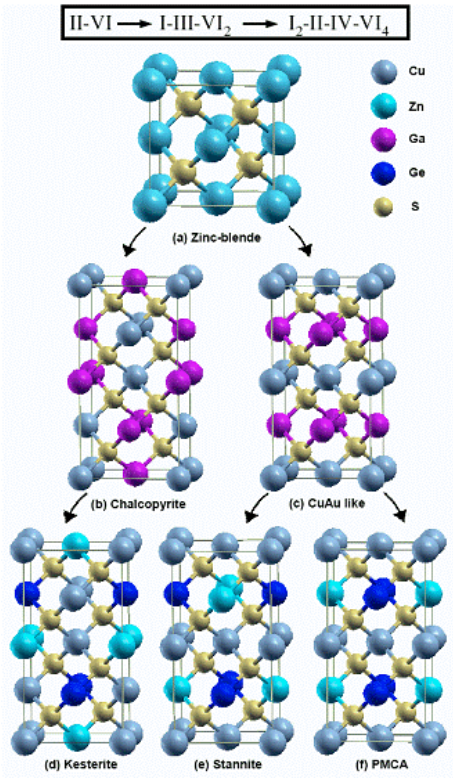

FIG. 1. Through cation site atomic mutation, we have systematically searched quaternary chacogenides for possible solar cell absorber applications. We show that the stable structures always obey the octet rule during mutation. For the intra-row cation mutation, chalcopyrite structure is the most stable for ternary compounds and kesterite structure has the lowest energy for the quaternary compounds. $Cu_2ZnGeSe_4$ is identified as the optimal material for solar cell absorber application [2].

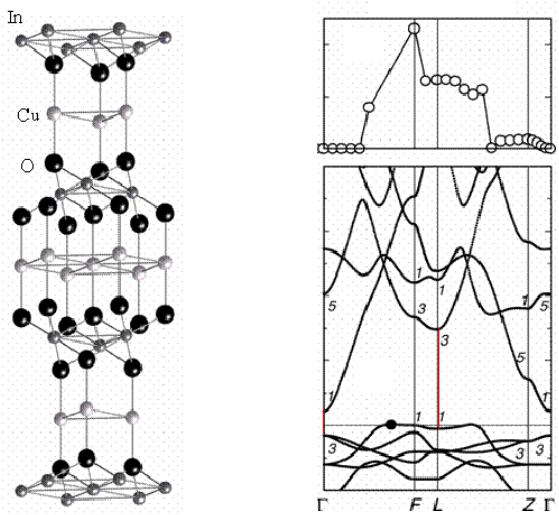

FIG. 2. Crystal and band structures of $CuInO_2$. We show that a bipolarly dopable TCO such as $CuInO_2$ should have a large optical band gap so it is transparent, but also a small fundamental band gap so it can be doped both p- and n-type [7].