DENSITY FUNCTIONAL THEORY-BASED STUDY OF Cu_2TiSnS_4 AND Cu_2VSnS_4 FOR PHOTOVOLTAIC APPLICATIONS

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I. INTRODUCTION

Cu_2ZnSnS_4 (CZTS) is a promising earth abundant and non-toxic intrinsic p-type semiconducting material [1]. However, similar radii of Cu and Zn atoms facilitates formation of anti-site defects which degrade performance of CZTS solar cells [2]. Thus, there is need to find an alternative to Zn to reduce cation disordering. In the present work, we fully replace Zn atoms in CZTS by Ti and V atoms and study the effects of the substitution on the band structure and stability of the alternative kesterite material using density function theory (DFT) [3].

II. METHODS AND RESULTS

The calculations have been performed by Vienna Ab initio Simulation Package (VASP). It has been found that upon Zn substitution by Ti in CZTS its band gap (E_g) decreases and shifts from direct to indirect compared to that of pristine CZTS (Fig. 1a-b). On the other hand, there is no E_g upon Zn substitution by V (Fig. 1c). The calculated binding energies of CZTS (10.16 eV), Cu_2TiSnS_4 (11.23 eV) and Cu_2VSnS_4 (11.52 eV) suggest high stability of the material after the Ti and V substitution.

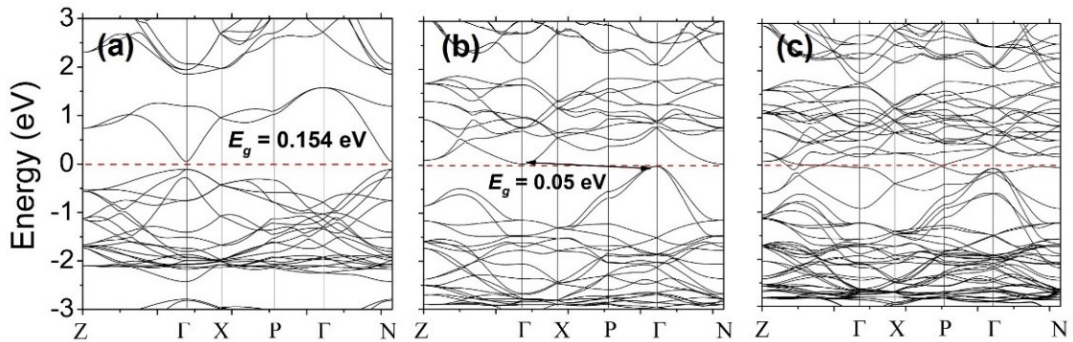

Figure 1. Band structure of (a) pristine CZTS, (b) Cu_2TiSnS_4, (c) Cu_2VSnS_4

III. CONCLUSIONS

In conclusion, Ti substitution enables to tune E_g and enhance thermodynamic stability of the material.

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