Properties of Natural Intermediate Band in Cu_2CdGeS_4 for Intermediate Band Solar Cells: A First-Principle Insight

Murugesan Rasukkannu [1], Dhayalan Velauthapillai [1], Ponniah Vajeeston [2]

[1]*Western Norway University of Applied Sciences, Department of Computing, Mathematics and Physics, Bergen, Norway*

[2]*Center for Materials Science and Nanotechnology, Department of Chemistry, University of Oslo, Oslo, Norway*

rmrmurugesh@gmail.com

Abstract

The development of intermediate band solar cells is an intermediate band in the band gap of the semiconductor, but it is generally produced artificially, which executes practical challenges on the synthesis side. Here, we found the natural intermediate band in the main band gap of Cu_2CdGeS_4 by first-principle calculations. Cu_2CdGeS_4 is I_2-II-IV-VI_4 group quaternary chalcogenide semiconductor, which had been proposed as promising light-absorber layer efficiency of Cu-based chalcogenide. For the first time, we found the isolated conduction band of Cu_2CdGeS_4 in the zincblende or wurtzite structure, which can be regarded as a natural intermediate band (partially filled) by employing a hybrid functional model. This evidence for the first time that absorption coefficient of both valance band to intermediate band and intermediate band to conduction band transition involving intermediate band are of significant by employing BSE method and corresponding to electronic transitions. The results imply that Cu_2CdGeS_4 being two-photon absorption in the visible light range. Additionally, the hole and electron effective masses of Cu_2CdGeS_4 are systematically studied using first-principle calculations. We show that Cu_2CdGeS_4 could make possible intermediate band solar cells of improved efficiency.