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Density functional theory study of copper zinc tin sulphide (Cu_2ZnSnS_4) doped with calcium and barium

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The sun is the most important source of renewable energy today. Producing energy from sunlight using cheap, abundant and non-toxic materials is considered a major challenge in the field of solar-electrical energy conversion. To harvest the solar energy, a thin film solar cell composed of the Cu_2ZnSnS_4 (CZTS) semiconductor is a candidate which can harvest as much energy as possible. Its advantages are optical direct band gap and high absorption coefficients. The structural, electronic and optical properties of doped CZTS will be calculated using the density functional theory (DFT) as implemented in the CASTEP codes. A new doping mechanism will be used to dope by the alkali earth metals, Calcium (Ca) and Barium (Ba). The dopants will be placed in the structure rather than replacing one of the atoms. Doping using the different elements is expected to improve the conversion efficiency of the CZTS based solar cells.

Key words: Cu_2ZnSnS_4, density functional theory, electronic properties, optical properties, doped and undoped Cu_2ZnSnS_4

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