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First-principles Study of Cu2ZnSnS4 Photovoltaic Absorber RYOJI ASAHI, AKIHIRO NAGOYA, Toyota Central R&D Labs., Inc., GEORG KRESSE, Universitat Wien — The quaternary semiconductor Cu2ZnSnS4 (CZTS) is a relatively new photovoltaic material whose constituents are non-toxic and abundant in the earth's crust. The highest conversion efficiency reported so far is 6.7%, demanding further improvement. The key computational issue is to predict optical properties as accurate as possible, which is not possible using conventional semi-local density functionals. To this end, we have employed the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional as implemented in the Vienna Ab-initio Simulation Packages (VASP) code, which allows us to obtain results in good agreement with the experimental data for the lattice constants and the band gap of CZTS [1]. We then predicted optical properties and determined the dominant optical transitions for solar-light absorption. The defect formation energies of CZTS were also calculated in the allowed range of the chemical potentials bound by the precipitation conditions of the metal-sulfides.

[1] J. Paier et al., Phys. Rev. B 79 115126 (2009).

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