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New quaternary semiconductor Cu_2MgSnS_4 and $Cu_2MgSnSe_4$ for photovoltaics[1] KINFAI TSE, Chinese Univ of Hong Kong, GUOHUA ZHONG, Chinese Academy of Sciences, Shenzhen, YIOU ZHANG, Chinese Univ of Hong Kong, XIAOGUANG LI, CHUNLEI YANG, Chinese Academy of Sciences, Shenzhen, JUNYI ZHU, Chinese Univ of Hong Kong, ZHI ZENG, Chinese Academy of Sciences, Hefei, ZHENYU ZHANG, University of Science and Technology of China, Hefei, XUDONG XIAO, Chinese Univ of Hong Kong — Element substitution of Zn by Mg and Ca is attempted to overcome the problem of potential fluctuation in Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$ (CZTSSe) due to prevalence of Cu_{Zn}+Zn_{Cu} defect complex. Through density function theory calculation with hybrid functional, we have shown that Cu_2MgSnS_4 and $Cu_2MgSnSe_4$ (CMTSSe) are stable with respect to secondary phases considered under suitable chemical potential. Stannite CMTSSe is thermodynamically more favorable over the kesterite structure. The alternating Cu and Mg/Sn cation layer of stannite structure may suppress the formation of Mg_{Cu} antisite due to large stress induced. The electronic and optical properties of CMTSSe are similar to that of CZTSSe with comparable absorption coefficient at the band-edge suggests CMTSSe to be a promising photovoltaic material.

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