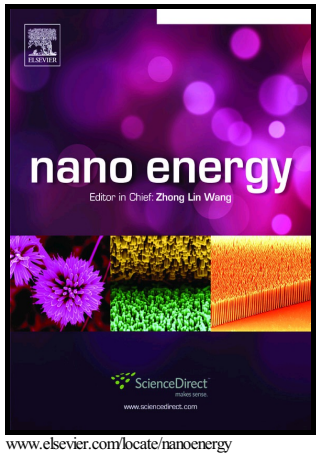

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Multi-cations Compound Cu_2CoSnS_4: DFT Calculating, Band Engineering and Thermoelectric Performance Regulation

Dan Zhang, Junyou Yang, Qinghui Jiang*, Zhiwei Zhou, Xin Li, Jiwu Xin, Abdul Basit, Yangyang Ren, Xu He*

State Key Laboratory of Material Processing and Die & Mould Technology, Huazhong University of Science & Technology, Wuhan 430074, P. R China

E-mail: jyyang@mail.hust.edu.cn, qhjiang@mail.hust.edu.cn

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Abstract

Owing to the advantage of low thermal conductivity, large Seebeck coefficient and multiple eco-friendly component constitution, Cu_2CoSnS_4 (CCTS) might be a promising thermoelectric material. DFT calculations reveal that the multiple valence bands can be utilized to obtain an enhanced Seebeck coefficient and an improved power factor, and the relatively low sound velocity in multi-cations-containing CCTS is responsible for the low thermal conductivity. Here, nano-sized CCTS sulfide has been facilely synthesized through mechanical alloying and then sintered via hot-pressing. Guided by the theoretical calculations, copper substitution is firstly adopted to regulate electrical properties and results in a highly improved power factor with an enhanced effective mass. Then, transition metal M (M = Mn, Fe, Zn) and Cu are co-doped at cobalt site to further regulate the TE performance of CCTS. As a consequence, a peak ZT value about 0.8 at 800K is achieved in the CCTS compound simply by Cu/Mn dual-doping due to the improved electrical properties by