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First-principles study of the thermoelectric properties of Cu2S KEENAN ZHUO, Georgia Institute of Technology, CHENG-RONG HSING, CHING-MING WEI, Institute of Atomic and Molecular Science, Academia Sinica, Taiwan, MEI-YIN CHOU, Institute of Atomic and Molecular Science, Academia Sinica, Taiwan and Georgia Institute of Technology — The mineral chalcocite, or copper sulphide (Cu₂S), is of interest as a thermoelectric material due to its abundance and non-toxic nature. Yet, the study of Cu₂S is complicated by the disordered phases (hexagonal and face-centered cubic) that it exists in at high temperatures. Here, we discuss our random structure search leading to the most stable structures. Based on these results, we report the thermoelectric properties of hole doped Cu₂S using first-principles calculations and Boltzmann transport theory. We show that a high Seebeck coefficient of over 200 μ V/K is achievable with hole doping levels up to 10²⁰ cm³ above 500 K.

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