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Thermoelectric Performance of Hole-Doped Cu_2O[1] XIN CHEN, DAVID PARKER, MAO-HUA DU, DAVID J. SINGH, Oak Ridge National Laboratory — We present an analysis of the thermopower and related properties of hole-doped Cu_2O using first-principles calculations and Boltzmann transport theory. Our results show that hole-doped Cu_2O has a high thermopower of above 200 μV/K with doping levels as high as 5.5×10^{20} cm^{-3} at 500 K, mainly attributed to the heavy valence bands of Cu_2O. The current theory suggests that hole-doped Cu_2O could be a good thermoelectric material. Future experiments are thus suggested to explore its thermoelectric potential for practical use in cooling and power generation applications.

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