

SUPPLEMENTARY INFORMATION

Bipolar effect in thermoelectric material CaMg_2Bi_2 by a first-principles study

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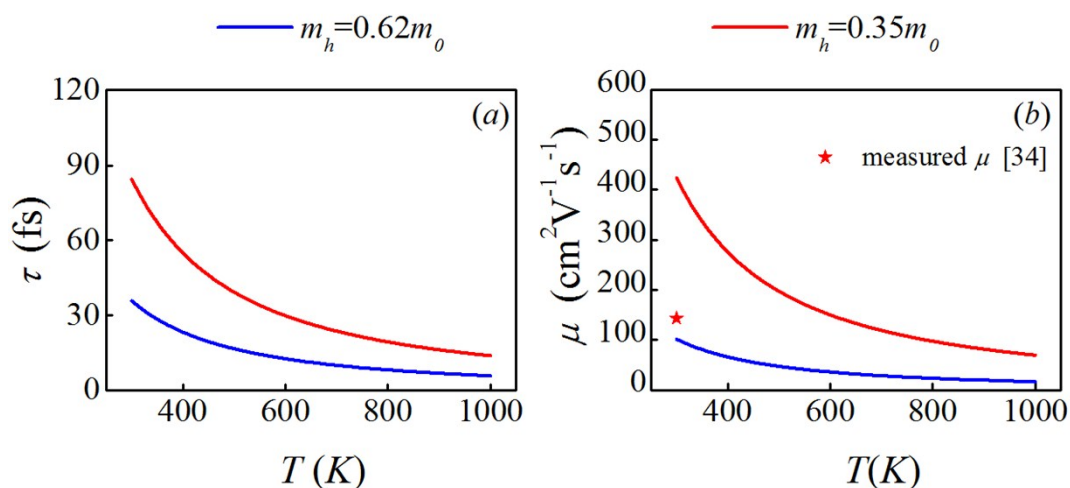


Figure S1. The calculated relaxation time τ (a), mobility μ (b) for the hole-type carrier. The red and blue lines respectively represent the calculated data using the effective mass $m_h=0.35m_0$, and $m_h=0.62m_0$, here m_0 is the electron mass. The measured mobility at room temperature is marked with a red star.

In this work, the relaxation time τ is calculated using the effective mass approximation based on the DP theory. The effective mass $m_h = 0.35m_0$ is obtained from the electronic structure data, which is lower than the experimentally estimated effective mass of $0.62m_0$. At 300K, the measured mobility μ is $\sim 143\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ as reported in Ref. [34]. The calculated mobility value is $\sim 420\text{cm}^2\text{V}^{-1}\text{s}^{-1}$. The difference comes from the fact that we only take into account of the acoustic phonon scattering, where experimentally more scattering sources exist,

including grain boundaries, lattice defects, and impurities etc. In order to better analyze the bipolar effect in CaMg_2Bi_2 , we take $m_h=0.62m_0$ in the present calculations.