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How optimizing a green promising thermoelectric materials? The case of Mg_2Si

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During the last years, thermoelectricity has attracted the attention because it is a potentially green energy. However, the commercially used thermoelectric materials contain toxic elements such as tellurium that is very rare element. In order to permit to thermoelectricity to contribute to advances in the search of green energy at reasonable costs, it is therefore necessary to find new thermoelectric elements based on abundant elements with low toxicity. Silicides are such compounds and the most promising family of this compounds are based on the semiconducting compound Mg_2Si that crystallizes in antifluorite structure. However, only n-type compounds based on Mg_2Si have high thermoelectric Figure of Merite ZT of about 1 at about 800 K that is similar to state-of-the art bismuth telluride compounds at room temperature [1]. But for practical use, we need to still improve the thermoelectric properties of these materials, especially for the p-type and to find how to obtain high thermoelectric performance in the case of the n-doping.

In the present communication, we present a combined theoretical and experimental study of the stability and thermoelectric properties of alloys based on Mg_2Si. This study, together with experimental studies in literature, confirms the possibility to obtain ZT = 1 for the n-doping and we also predict that similar ZT could also be obtained for the p-doping. However, as the most favorable point defects are interstitial Magnesium atoms acting as donors, it is very difficult in practice to get the good doping level for reaching this high ZT in the case of p-doping. For overwhelming this problem, we have also studied the solid solution Mg_2Si-Mg_2X (X = Ge, Sn) that present some miscibility gap, at least for the case of Sn [2] and our calculations suggest new directions for resolving the problem of p doping, related to the change of stability of the defects when Ge or Sn are substituted to Si.

Références

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