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First-principle study of thermoelectric properties of impurity-doped magnesium silicide Mg2Si HIROKI FUNASHIMA, Osaka University — The electronic structure and the thermoelectric properties of Mg_2Si doped with several dopants, Al, Bi, Sb, and Zn, are theoretically examined using a first-principles calculation method. Mg_2Si is a promising thermoelectric material that is functional in the temperature range from 500 to 800 K. Therefore, it is expected to be useful for recovering waste heat from exhaust gas in automotive applications, incinerators, and boilers. Moreover, this material has several desirable attributes with respect to cost and environmental protection: it is cheap, nontoxic, and composed of elements abundant on Earth. These advantages are important for practical usage in thermoelectric applications. Impurity doping is a well-established way to improve the thermoelectric performance of Mg_2Si. Undoped Mg_2Si crystals have n-type conductivity, but they can be doped with both n- and p-type impurities. A fundamental understanding of the relationship between impurity doping and the thermoelectric properties of Mg_2Si will allow us to provide theoretical guidelines for further development of this material. As an effort toward this goal, we present here the band structure of Mg_2Si using the full-potential linearized augmented plane-wave (FLAPW) method based on LDA/DFT and the conductivity.

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