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Thermal and Electric Properties of the $FeAs_{2-x}Sb_x$ (x=0, 1, or 2) Marcasite Compounds from First Principles

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Thermoelectric energy conversion has been considered as one piece of the future solution to the energy crisis for a long time. In thermoelectric energy conversion, thermoelectric materials, which exhibit strong coupling between heat flow and electric current, are used to convert thermal energy into electrical energy and vice versa. Hence, thermoelectric devices can be potential and present applications for both thermoelectric generation and cooling system. There are significant demands for thermoelectric materials that can be used for environment-friendly cooling applications that need to be met. A few recent studies reported thermoelectric properties of the $FeAs_{2-x}Sb_x$ (x=0, 1, or 2) marcasite compounds, which has a potential for becoming a good thermoelectric material for low-temperature cooling applications. The compound can be more environment-friendly and more economically viable than other competing materials, for the composition does not involve rare and expensive element like Te or Pt. In this study, we investigate thermoelectric properties of the $FeAs_{2-x}Sb_x$ (x=0, 1, or 2) marcasite compounds by first-principles calculations in order to demonstrate the feasibility for the use in practical cooling applications. Electronic band structures and density of states are constructed from DFT (density functional theory) calculations, from which electrical properties, including the Seebeck coefficient and the electrical conductivity, are estimated. At the same time, vibrational characteristics are investigated through DFPT (density functional perturbation theory) calculations, from which the thermal conductivity is estimated using semiempirical formulae and the Grüneissen parameters of the compound obtained at the level of the QHA (quasi-harmonic approximation).