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The calculation of thermoelectric properties of GeSi alloy

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Abstract

The electronic structure and thermoelectric properties, including thermal conductivity, electrical conductivity and Seebeck coefficient, of $Ge_{(1-x)}Si_x$ alloy in various composition of x were calculated by means of the principle calculation on Generalized Gradient Approximation (GGA) , packaged in Abinit code, and the semi-classical Boltzmann transport theory, packed in the BoltzTrap respectively. The $Ge_{(1-x)}Si_x$ alloy was modeled as 1x1x2 super-cell in diamond structure which consists of 16 atoms. The germanium (Ge) and silicon (Si) affect the electronic and thermoelectric properties that were studied by comparing the results of pure silicon, pure germanium and alloys. The results indicated that the energy band gap of alloy will decrease when the Ge of alloy increase. For thermoelectric properties, the result showed that the figure of merit (ZT) of silicon-rich doped with germanium atom is higher than pure silicon, pure germanium, germanium-rich doped with silicon atom, and GeSi alloy in zinc-blend structure. This is because of the Ge-atom-defect which plays an important role as a heavy-ion phonon scatter in reducing thermal conductivity.

Keywords:

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Stability Investigation of Hesperetin Loaded Nanocarrier

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Abstract

The aim of this study was to investigate the stability of hesperetin loaded nanostructure lipid carriers (NLC) and solid lipid nanoparticles (SLN). NLC and SLN were produced using high shear method and their stability over 30 days was evaluated based on hesperetin leakage, size and zeta potential. In spite of different advantages, NLC and SLN were not physically stable due particle aggregation. However Developed nanocarriers did not show any hesperetin leakage during 30 days.

Keywords: hesperetin; nanostructure lipid carriers; solid lipid nanoparticles; stability