Conference Proceedings – Volume 1010 MSF, Materials Science Forum 2020, Pages 334 – 338

Thermoelectric properties of sm doped camno3 using density functional theory method

Abstract

The electronic structure and thermoelectric properties of CaMnO3 doped with 8% and 17% f block element Sm using first principles calculations and semi-classic Boltzmann theory were presented in this paper. The G-type AFM phase is most stable among five phases for CaMnO3, however, with 8% and 17% Sm doping, these compounds became nonmagnetic phases. CaMnO3 calculated electronic band structure shows an indirect band gap of 0.523 eV, which is underestimated by the density functional theory (DFT) calculations but the band gap explains the semiconducting behavior. However, with 8% and 17% Sm doping, the electronic bandstructure of these compounds exhibit metallic behavior, with Sm 4f and Mn 3d electrons contributing to conduction band, increasing the magnitude of conductivity for doped compounds. All temperature dependence Seebeck coefficient plots show n-typed conduction for all compound with reduced magnitude of Seebeck coefficient for doped compounds. The temperature dependence thermal conductivity plot shows overall thermal conductivity is reduced in Sm doped compound. CaMnO3 with 17% Sm doping exhibit much higher ZT of 0.32 at 800 K showing enhanced thermoelectric properties at high temperature and suitability or high temperature energy conversion devices.

Keywords

Density functional theory; First principles; Thermoelectric