

Abstract Submitted
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Enhancement of Thermoelectric Properties of Lead Selenide by Doping¹ HAOWEI PENG, JUNG-HWAN SONG, A. J. FREEMAN, Northwestern University — Lead chalcogenide materials are very important in thermoelectric investigations. Recently, it is reported that Tl doping in PbTe can greatly enhance the figure of merit (ZT) of PbTe,² which can be mainly attributed to resonance states near the Fermi level. PbSe is also a good candidate as a thermoelectric material since it has a high melting temperature and low thermal conductivity (1.6 W/mK).³ Here we present a theoretical study of the electronic structures, formation energies, and transport properties of PbSe doped with various impurities such as Ga, In, Tl, As, Sb, and Cd using the highly precise FLAPW method.⁴ Our calculated formation energies indicate that As prefers Se sites rather than Pb sites due to atom size mismatch, but Sb has no apparent preferable sites. Based on the analysis of the densities of states, PbSe with Tl and Cd doped on the cation sites are good candidates for thermoelectric applications as p-, and n-type materials. We also discuss the possible enhancement of thermoelectric properties in terms of optimal carrier concentrations.

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²J. P. Heremans, et al, *Science*, **321**, 554 (2008)

³S. Ahmad, et al., *Phys. Rev. B* **74**, 155205 (2006)

⁴Wimmer, Krakauer, Weinert, Freeman, *Phys. Rev. B*, **24**, 864 (1981)

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