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Engineering lattice vibrations of chemically doped SnSe for thermoelectric applications - ab initio calculation[1] TREVOR FITZPATRICK, Wabash College, HANSIKA SIRIKUMARA, THUSHARI JAYASEKERA, Southern Illinois University — Due to the efficiency constraint of the thermoelectric conversion process, there is an intense search for highly efficient thermoelectric materials. Recent findings among the scientific community of the extreme thermoelectric properties of the earth-abundant, non-toxic SnSe compound has provided experimental evidence of an outstanding figure of merit. Our work explores how to engineer the thermoelectric properties of SnSe by controlled chemical doping using density functional theory. We considered both Sn-site doping, Se-site doping as well as Sn and Se codoping of SnSe. By exploring vibrational properties, our work shows that codoping is more favorable over singular Sn-site and Se-site doping in SnSe. This suggests future experiments should focus on similar forms of doping.

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