Abstract Submitted
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First-principles study on the high thermoelectric efficiency originating from "pudding-mold" bands in n- and p-type SnSe HITOSHI MORI, HIDETOMO USUI, MASAYUKI OCHI, KAZUHIKO KUROKI, Department of Physics, Osaka University — The performance of thermoelectric conversion is evaluated by the dimensionless figure of merit $ZT = (\sigma S^2/\kappa)T$, where σ, S, κ, and T are the electrical conductivity, thermopower, thermal conductivity, and temperature, respectively. Recently, it has been experimentally found that SnSe exhibits a high ZT=2.6 at 923 K [1]. Its high ZT is mainly due to the ultralow thermal conductivity. Some theoretical studies have shown that the ultralow thermal conductivity originates from strong anharmonicity of the phonons, and suggested that ZT could be further increased by doping electrons or holes[2,3]. In the present study, we analyze the thermoelectric properties of the carrier-doped SnSe to reveal the origin of its even higher performance. Using the first-principles calculation and adopting the Boltzmann equation, we obtain the electrical conductivity and the thermopower. We find that the pudding-mold-shaped band structure [4] enhances its thermoelectric performance not only in the hole-doped [2] but also in the electron-doped regime, where the Bloch states at the Fermi level originate from Se p_x in the former, and Sn p_y in the latter. [1] L.-D. Zhao *et al.*, Nature **508**, 373 (2014). [2] K. Kutorasinski *et al.*, Phys. Rev. B **91**, 205201 (2015). [3] R. Guo *et al.*, Phys. Rev. B **92**, 115202 (2015). [4] K. Kuroki and R. Arita, J. Phys. Soc. Jpn. **76**, 083707 (2007).

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