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Theoretical Study of Layered Oxychalcogenides as Thermoelectric Materials HIROKI FUNASHIMA, Osaka Univ — In order to restrain global warming and realize a sustainable global energy system, the researches of various energy resources are done. In these various energy resources, attracted technology is thermoelectric technology. Recently Layered oxychalcogenides has interesting properties useful for new type thermoelectric materials. Firstly, from DFT and DFPT calculations, we performed the electronic structure calculation and the thermal structure calculation about layered oxychalcogenides. In addition, we calculated thermoelectric properties Blotch-Boltzmann equation, semi-classically. We indicate the mechanism behind the high power factor from calculation about the transport properties. The key to understanding the power factor is that different effective masses contribute to different transport phenomena in the crystal. The discrepancy between the effective mass for the conductivity and the thermoelectric power showed that the conductivity and thermoelectric power are conveyed by electrons with different effective masses in the Brillouin zone. In point of view the thermal conductivity κ, we discuss the electronic part κ_{el} from Bloch-Boltzmann equations, and κ_{ph} from DFTP calculations.

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