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Electronic Structure and Thermoelectric properties of (LaO)x(MCh)y HIROKI FUNASHIMA, HIROSHI KATAYAMA-YOSHIDA, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka Univ. — (LaO)MCh (M=Cu,Ag,Au, Ch=S,Se,Te) are known as transparent narrow gap p-type semiconductor, which give an excitonic absorption/emission near the band edge even at room temperature. These compounds have P4/nmm structure and can oxide natural superlattice semiconductor. In this paper at first, we calculated band structure for these compounds, using FLAPW based on LDA/DFT. In our results, these compounds have large anisotropy k_z direction. On Λ, V, and W axises, dispersion curves are very flat. W analyze the electronic structure by group theory. Secondly, we calculated conductivity tensor and Seebeck coefficient using Bloch-Boltzmann Equation semi-classically. Bloch-Boltzmann equation shows that in small dispersion so-called flat band structure, shape of Fermi-surface increase as temperature increase, dramatically, in the result these compounds have large Seebeck-coefficient. As mentioned, we showed that because these compounds have flat-band structure in a direction toward k_z, these compounds have large Seebeck coefficient. At the same time, these compounds have a small hole-pocket in valence band, thus these compounds have good electric conductivity. Finally, we changed chalcogen Ch(=S, Se,Te) and will suggest new-generation high-efficie

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