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First principles approaches for the structure searching in thermoelectric Ge-Ag-Sb-Te alloys HIKARI SHINYA, HIROKI FUNASHIMA, AKIRA MASAGO, TETSUYA FUKUSHIMA, HIROSHI KATAYAMA-YOSHIDA, Osaka Univ — Since the discovery of a discontinuous decreasing of the thermal conductivity without changing of the electric conductivity in quaternary $AgSbTe_2$-GeTe (TAGS) alloys by Skrabek and Trimmer[1], the TAGS alloys have attracted much attention as the good thermoelectric materials. However, the mechanism of the dramatic change of thermal conductivity has yet to be understood, and even the crystal structures of the TAGS alloys are still under discussion. In this talk, to shed light on this problem, we investigate the electronic structures of Ag and Sb doped GeTe by first-principles calculations[2], and also perform the structure searching in the quaternary TAGS alloys by a multicomponent cluster expansion method[3]. We will discuss an important correlation between the crystal structure and the anomalous thermal conductivity based on our calculation results. [1] E. Skrabek and D.Trimmer, U.S. Patent No. 3945855 (23 March 1976). [2] G. Kresse and D. Joubert, Phys. Rev. B, 59, 1758 (1758). [3] A. van de Walle et al., CALPHAD: Comput. Coupling Phase Diagrams Thermochem. 26, 539 (2002).

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