Strong Correlation Effect by the Rare Earth Substitution on Thermoelectric Material Bi_2Te_3 ; in GGA+U Approach

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Abstract: Thermoelectic properties of the typical thermoelectric host materials, the tellurides and selenides, are known to be noticeably changed by their volume change due to the strain [1]. In the bismuth telluride (Bi_2Te_3) crystal, a substitution of rare-earth element by replacing one of the Bi atoms may cause the change of the lattice parameters while remaining the rhombohedral structure of the host material. Using the first-principles approach by the precise full potential linearized augmented plane wave (FLAPW) method [2], we investigated the Ce substitution effect on the thermoelectric transport coefficients for the bismuth telluride, employing Boltzmann's equation in a constant relaxation-time approach fed with the FLAPW wave-functions within the rigid band approximation. Depending on the real process of re-arrangement of atoms in the cell to reach the equilibrium state, $CeBiTe_3$ was found to manifest a metal or a narrow bandgap semiconductor. This feature along with the strong correlation effect originated by the 4f states of Ce affect significantly on the thermoelectric properties. We showed that the position of the strongly localized f-states in energy scale (Fig. 1, f-states are shaded) was found to alter critically the transport properties in this material suggesting an opportunity to improve the thermoelectric efficiency by tuning the external strain which may changing the location of the f-sates.

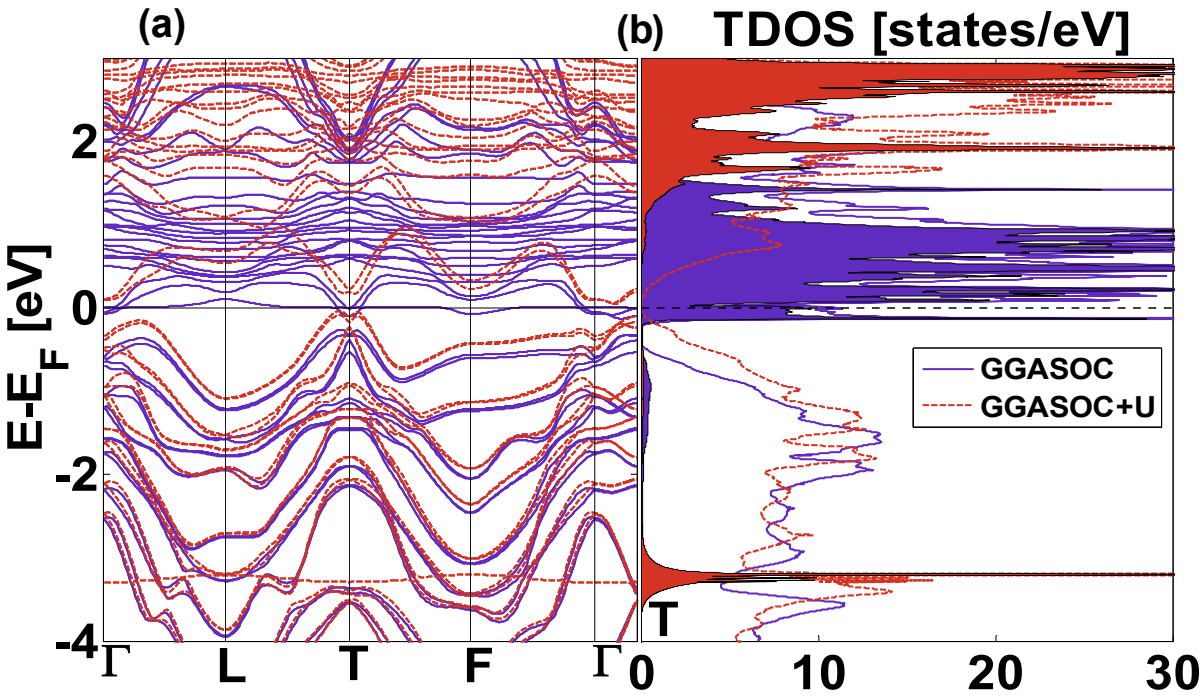

Fig. 1. (a) Band structure and (b) DOS within GGA-SOC (solid violet line) and GGASOC+U (dash orange line) calculations with the shaded f-states, respectively

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참고문헌

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