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First principles Study on Transparent High-T_c Superconductivity in hole-doped Delafossite CuAlO₂ AKITAKA NAKANISHI, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — The CuAlO₂ is the transparent *p*-type conductor without any intentional doping. Transparent superconductivity and high thermoelectric power are suggested in *p*-type CuAlO₂ [1]. Katayama-Yoshida *et al.* proposed that it may cause a strong electron-phonon interaction and a superconductivity. But, the calculation of superconducting critical temperature T_c is not performed. We performed the first principles calculation about the T_c of hole-doped CuAlO₂ by shifting the Fermi level rigidly. In lightly hole-doped CuAlO₂, the Fermi level is located at Cu and O anti-bonding band. The electrons of this band strongly interact with the A₁L₁ phonon mode because the direction of O-Cu-O dumbbell is parallel to the oscillation direction of the A₁L₁ phonon mode. As a result, T_c of lightly hole-doped CuAlO₂ is about 50 K. We also discuss the materials design to enhance the T_c based on the charge-excitation-induced negative effective U system.

[1] H. Katayama-Yoshida, T. Koyanagi, H. Funashima, H. Harima, A. Yanase: Solid State Communication **126** (2003) 135.

[2] A. Nakanishi and H. Katayama-Yoshida: Solid State Communication, in printing. (arXiv:1107.2477v3)

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