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Enhancement mechanisms of two-particles exchange scattering processes in single-layer cuprate superconductors SHINGO TERANISHI, SATOAKI MIYAO, KAZUTAKA NISHIGUCHI, KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka University — To estimate effective in-plane exchange interactions of a CuO_2 layer, we applied self-consistent exact-exchange calculations for several single-layered cuprate superconductors, and explored material dependence of the effective super-exchange processes mediated by all relevant orbitals of the real materials. The effective exchange is enhanced owing to low-lying energy levels originated from the buffer layers of Hg1201 ($T_C \simeq 100\text{K}$), while the effect is smaller for Tl1201 ($T_C \simeq 50\text{K}$) than mercury compounds. The case of the Tl2201 is intermediate. The effective exchange is relevant in the strong-correlation mechanism of the superconductivity in cuprate, which may reveal the material dependence found in real experiments.

Shingo Teranishi
Graduate School of Engineering Science, Osaka University

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