Two-orbital view on the origin of the material dependence of T_c in the single-layer cuprates

H. Sakakibara[a], H. Usui[b], K. Kuroki[a], R. Arita[c], and H. Aoki[d]

[a]Department of Engineering Science, University of Electro-Communication, Tokyo, Japan
[b]Department of Applied Physics, University of Electro-Communication, Tokyo, Japan
[c]Department of Applied Physics, University of Tokyo, Tokyo, Japan
[d]Department of Physics, University of Tokyo, Tokyo, Japan

While the significant material dependence of T_c even within the single-layer high T_c cuprates has remained a basic puzzle, a recent paper[1] has demonstrated that the usually considered $d_{x^2-y^2}$ orbital is in fact mixed with the d_{z^2} orbital around the Fermi energy, which is shown to affect T_c in the spin-fluctuation mediated pairing with a two-orbital model that incorporates d_{z^2} as well as $d_{x^2-y^2}$. There, the energy offset (ΔE) between the two orbitals has been shown to govern the extent of the d_{z^2} mixture, hence T_c. In the present study, we extend this work to identify which key factors determine ΔE in the cuprates, focusing on the structural difference among broader (La, Hg, Bi, and Tl) single-layer cuprates. We have revealed that the apical oxygen height ($h_{\rm O}$) above the CuO_2 plane and the distance (d) between the CuO_2 planes are the important parameters that determine ΔE, thereby causing the material dependence of T_c. This picture enables us to capture the T_c variation among the single-layered cuprates in a simple lattice parameter space.

[1]H. Sakakibara *et al.* Phys. Rev. Lett. **105**, 057003(2010).