

Ti dxy orbitals in STO and virtual hopping

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The lowest energy conduction band in STO along $\Gamma - Z$ is one dominated by Ti dxy orbitals. It also has very small dispersion with an effective mass of about 5 times the usual electron mass (as per Hanghui's calculations). After thinking for a while, I couldn't not find any atomic states and hopping among them to provide any dispersion for this state within the usual tight-binding basis of Ti d states and oxygen p states. This is unchanged by including oxygen and Sr s states again as per symmetry. Also, I did a short tight-binding calculation based on the perovskite book we keep looking at confirming this point. Also, as per Hanghui, the direct Ti-Ti hopping elements are about 10-100 times too small to give the observed dispersion.

The only way I could see coupling would be through some other dxy type orbitals on the oxygen or the Sr or both. How does this work? Here is a simple model shown in the figure. Basically, we have the Ti dxy states at some energy $-V_0$ and some other unknown states at energy $+V_0$ and they are coupled by hopping element t . All other hoppings (e.g. Ti-Ti) are

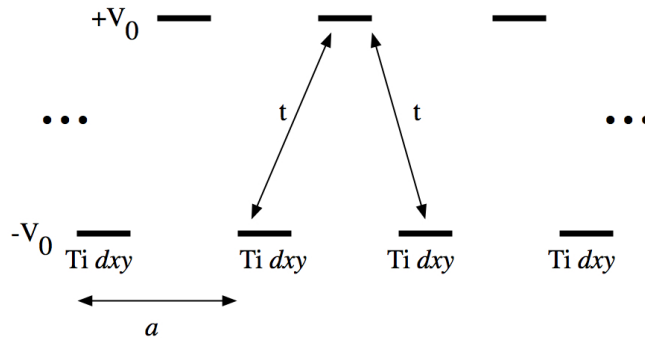


Figure 1: The Ti dxy states are at energy $-V_0$ and some other orbitals are at higher energy $+V_0$. The only non-zero hopping is between the Ti dxy and the other orbitals and is of strength t . The lattice constant is a between pairs of dxy orbitals while the other orbitals are halfway and $a/2$ away from the dxy .

set to zero. Bloch's theorem gives the 2×2 tight-binding Hamiltonian

$$\begin{pmatrix} -V_0 & 2t \cos(ka/2) \\ 2t \cos(ka/2) & +V_0 \end{pmatrix}$$

which has band energies

$$E_{\pm}(k) = \pm \sqrt{V_0^2 + 4t^2 \cos(ka/2)^2}.$$

The low energy band is the one dominated by Ti dxy . For a weak dispersion, we can Taylor expand and use $\cos(x/2)^2 = (1 + \cos(x))/2$

$$E_-(k) \approx -V_0 - \frac{2t^2}{V_0} \cos(ka/2)^2 = -V_0 - \frac{t^2}{V_0} - \frac{t^2}{V_0} \cos(ka).$$

This result can also be gotten from second order perturbation theory.

The point is that the result looks exactly like what we would have gotten by only considering the linear chain of Ti dxy alone with a hopping of $t' = -t^2/(2V_0)$ between them. So the virtual second order hopping through the high energy state gives an effective hopping for the Ti dxy manifold. (The result holds for the high energy state as well.)