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# Effect of Hole Doping on the Electronic Structure of Tl2201

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We discuss doping dependencies of the electronic structure and Fermi surface of the monolayer  $\text{Tl}_{2-x}\text{Cu}_x\text{Ba}_2\text{CuO}_{6+\delta}$  (Tl2201). The TlO bands are found to be particularly sensitive to doping in that these bands rapidly move to higher energies as holes are added into the system. Such doping effects beyond the rigid band picture should be taken into account in analyzing and modeling the electronic spectra of the cuprates.

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The Fermi surface (FS) of  $\text{Bi}_{2-x}\text{Pb}_x\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  (Bi2212) predicted by band theory is well-known to display Bi-related pockets around the  $M(\pi, 0)$ -point, which have never been observed experimentally. We have shown recently<sup>1</sup> that when the effects of hole doping via Pb/Bi substitution or by adding excess oxygen are included, the BiO pockets are lifted above the Fermi energy ( $E_F$ ). With decreasing hole doping the BiO bands drop below the  $E_F$  and the system self-dopes below a critical hole concentration in the sense that further reduction in hole content no longer reduces the doping of the  $\text{CuO}_2$  planes. The aforementioned lifting of BiO pockets is a consequence of substantial Coulombic effects which come into play due to rearrangement of charges with changing hole concentration in the system. Ref.<sup>1</sup> presents detailed results on Bi2212 and provides more generally a first-principles route for exploring doping dependencies of electronic structures of the cuprates. Here we extend the discussion of Ref.<sup>1</sup> to consider doping effects in monolayer Tl2201.

Insofar as technical details are concerned, we have employed both the Korringa-Kohn-Rostoker (KKR) and linear augmented plane wave (LAPW) full potential band structure methodologies where all electrons are treated self-consistently<sup>2,3</sup>. The KKR scheme is well known to be particularly suited for a first-principles treatment of the electronic structure of substitutionally disordered alloys. Effects of hole doping were included within the framework of the virtual crystal approximation (VCA) which, as discussed in Ref.<sup>1</sup>, is expected to provide a reasonable description of the cation-derived bands near the  $E_F$  in the cuprates<sup>4</sup>. The tetragonal lattice data of Ref.<sup>5</sup> for an overdoped sample of Tl2201<sup>5,6</sup> was employed in the computations.

Fig. 1(a) shows the familiar band structure of undoped (half-filled,  $x = 0.0$ ) Tl2201. It displays the CuO band characteristic of the cuprates, which lies at  $\approx -1.3$  eV at  $\Gamma$ , yields the van Hove singularity (VHS) at  $\approx -0.5$  eV around the  $M(\pi, 0)$ -point, and forms along the  $M(\pi, 0) - X(\pi, \pi) - \Gamma$  line the non-symmetric inverted parabola. In addition to this CuO band, a second band, which is TlO-related, is seen to drop below the  $E_F$  at  $\Gamma$ , giving rise to a  $\Gamma$ -centered electron pocket, which has not been observed experimentally<sup>7,8</sup>. The problem is similar to that of BiO pockets noted above in connection with Bi2212 except

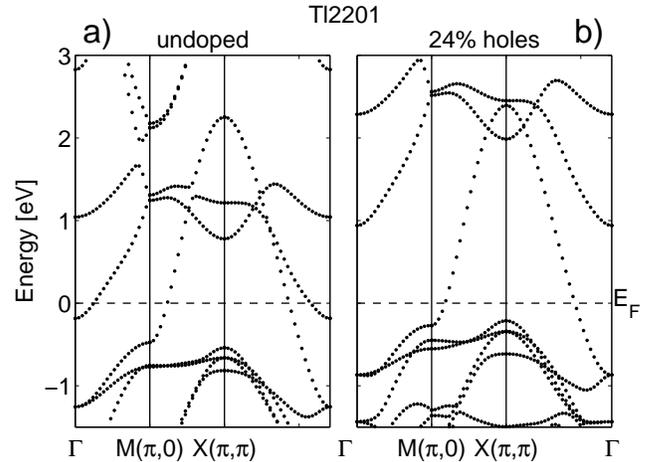


FIG. 1: Band structures of (a) undoped and (b) 24% hole doped Tl2201 along the main symmetry directions in the 2D Brillouin zone of the tetragonal lattice.

that here the pocket is centered around the  $\Gamma$  rather than the  $M(\pi, 0)$ -point.

Fig. 1(b) presents results for 24% hole doped Tl2201, where the effects of doping have been taken into account. The TlO band has now moved  $\approx 0.9$  eV above the  $E_F$  and the TlO pocket of Fig. 1(a) has disappeared from the electronic structure at an intrinsic level. At 24% hole doping, the rigid band shift (lowering) of the  $E_F$  will also empty the pocket<sup>8</sup>, but the present calculations show that this pocket will be removed very rapidly with doping as the TlO band moves to higher energies. Such an effect of doping beyond the rigid band model is less dramatic on the CuO band, although the CuO band also undergoes change in shape in that it narrows slightly with doping.

We comment briefly on our theoretical predictions in relation to relevant experimental results on overdoped Tl2201 single crystals. The shape and three-dimensionality of the FS derived from the band structure of Fig. 1(b) is in general accord with that reported in Ref.<sup>7</sup> via angular magnetoresistance oscillation (AMRO) measurements, including delicate variations in the shape of the 3D FS half-way between nodal and antinodal di-

rections, as well as with the angle-resolved photoemission (ARPES) results of Ref.<sup>8</sup>. However, even though the general shape and the 3D nature of the FS is captured by LDA, the theoretical FS is more squarish than the experimental one (i.e. closer to  $X$  in  $M-X$  direction and closer to  $\Gamma$  in  $\Gamma-X$  direction), possibly reflecting strong correlation physics beyond the conventional picture. Notably, the ARPES lineshapes for emission from the  $E_F$  in Tl2201 show relatively little broadening even in the antinodal region<sup>8</sup>, indicating that interlayer coupling effects in Tl2201 are smaller than in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO)<sup>9,10</sup>.

In summary, we have shown with the example of Tl2201 that the electronic structures and Fermi surfaces of the cuprates possess significant doping dependencies resulting from generic Coulombic effects that come into play as the electronic system rearranges itself with chang-

ing hole content, and that these effects are particularly pronounced on the cation derived bands (e.g. the TlO states in the case of Tl2201). The rigid band model, where one assumes the band structure to be independent of doping, has usually been the basis for discussing doping evolution of the electronic spectra of the cuprates in much of the existing literature. Our study shows that the rigid band model is fundamentally flawed and that doping effects on the electronic structure beyond the rigid band model should be accounted for in analyzing and modeling cuprate physics.

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