

Han and Savrasov Reply: In Singh's Comment [1] two statements are made regarding our Letter [2]: (a) Local density approximation (LDA) based calculations of doped Fe_{1+x}Te do not show the Fermi surface nesting at $(\pi, 0)$ when ~ 0.5 electrons is added per Fe (upward energy shift by ~ 0.4 eV) and show it only when ~ 1 electron is added per Fe (upward energy shift by ~ 0.7 eV) using rigid band approximation (RBA); (b) coherent potential approximation (CPA) calculations of doped FeTe do not show nesting at $(\pi, 0)$ at those dopings.

In regard to (a), we appreciate this discrepancy being pointed out to us, and indeed discovered “a factor of 2” error in extracting the doping in our original publication [2]. However, as we discuss below, the numbers deduced from LDA cannot be trusted due to correlation effects; therefore, the detailed quantitative analysis in Singh's Comment cannot be taken seriously into account for this system. We have already pointed out earlier [3] that LDA has an unprecedented error in determination of the z structural position of anion in pnictides. This, in particular, may lead to a 20% uncertainty in determining the density of states near the Fermi level. A different and possibly much larger source of error lies in the fact that there is a non-trivial frequency and orbital dependent self-energy correction to LDA. For example, previous LDA + dynamical mean field theory (DMFT) calculations [4] found band mass enhancements m/m_{LDA} to be between 2 [5] to 5 [4]. Angle resolved photoemission (ARPES) experiments show $m/m_{\text{LDA}} \approx 2$ for pnictides [6] while the situation is controversial for chalcogenides. Xia *et al.* [7] reported m/m_{LDA} in Fe_{1+x}Te similar to pnictides which, however, contradicts with the specific heat coefficient [8] by a factor of 4. A recent publication [9] finds much larger and anisotropic mass enhancements $\approx 6\text{--}23$ in $\text{FeSe}_{0.42}\text{Te}_{0.58}$ which also agrees much better with the Sommerfeld coefficient of Ref. [8]. On top of that the order of the bands near the Γ point seen by this ARPES experiment is in accord with LDA calculations for FeSe but not for FeTe. The fact that chalcogenides are more correlated than pnictides is also evident from comparative analysis of low energy model Hamiltonians derived by a first-principles electronic structure calculation [10].

The effect of correlation in the vicinity of the Fermi energy leads to the self-energy correction for the electron in the form $\Sigma_{\alpha}(\omega) = \Sigma_{\alpha}(0) + \omega(1 - z_{\alpha}^{-1})$, where z_{α} is the quasiparticle residue. Therefore, it is clear that the precise value of the energy shift necessary to change the topology of the Fermi surface depends on the mass enhancement and the value of 0.7 eV extracted from LDA is incorrect. For example, a mass enhancement of 10 would assume an upward energy shift by merely 0.07 eV to produce $(\pi, 0)$ nesting. A different consideration applies to the error in a number of electrons because isotropic mass enhancement alone will not affect the level of doping needed to change the Fermi surface due to Lattinger's theorem. In this regard, if the

mass enhancement is fairly band independent as it was seen in LDA + DMFT calculations for pnictides, the same value of ~ 1 electron per Fe would be needed. However, the situation may change since strong orbital dependence in the mass enhancement was recently reported together with the indication that some orbital dependent shift $\Sigma_{\alpha}(0)$ is needed to account for the correct order of the bands [9]. Under this circumstance, the Lattinger theorem does no longer hold and the value of doping needed to switch to the $(\pi, 0)$ nesting will be smaller.

In regard to comment (b), it is interesting but needs further study in its relevance to the physics of these systems. We would like to point out two things: first, several ARPES studies of doped Fe superconductors appeared in the literature; they may not see a disorder oriented broadening of the Fermi surfaces as reported by this CPA calculation. Second, a recent supercell study [11] concluded that virtual crystal approximation (VCA) is adequate to model the doping. We have performed our own VCA calculations, assuming a uniform positive background compensating for extra electrons, and verified that while there are important changes in band dispersions in the vicinity of Fermi level, the topology of the Fermi surface does follow the rigid band analysis of our original work and $(\pi, 0)$ nesting is still present.

To summarize, inclusion of correlation effects affects quantitatively the agreement with experiment as far as the value of energy shift and the level of doping is concerned, and our original statement that nesting at $(\pi, 0)$ can be responsible for magnetic behavior of FeTe is hereby reinstated.

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Received 19 January 2010; published 4 March 2010

DOI: [10.1103/PhysRevLett.104.099702](https://doi.org/10.1103/PhysRevLett.104.099702)

PACS numbers: 74.70.-b, 71.18.+y, 71.20.-b, 75.25.-j

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