Comment on "Doping Driven (π, 0) Nesting and Magnetic Properties of $Fe_{1+x}Te$ Superconductors"

In a recent Letter [1], Han and Savrasov described the changes in the electronic structure and magnetic properties of $Fe_{1+x}Te$ as a function of x using the full-potential, linear muffin-tin orbital (FP-LMTO) method within the rigid-band approximation (RBA). In particular, they used the electronic structure of FeTe and RBA to study the band structure, density of states (DOS), and Fermi surface (FS) of $Fe_{1.068}Te$ (or $Fe_{1.063}Te$) and $Fe_{1.141}Te$. They find that the excess Fe drives (π, π) FS nesting in FeTe to a (π, 0) nesting in $Fe_{1.068}Te$.

In this Comment, using the Korringa-Kohn-Rostoker coherent-potential approximation method in the atomic-sphere approximation [2] (KKR-ASA CPA) to describe the effects of disorder due to excess Fe in FeTe alloys, we show that (i) the rigid-band approximation is inadequate to describe the effects of disorder and its application leads to an incorrect description of the underlying physics, and (ii) the rigid-band energy shift of ~0.76 eV for going from FeTe to $Fe_{1.068}Te$ (or $Fe_{1.063}Te$), as obtained in Ref. [1], is inconsistent with our FP-LMTO as well as the KKR-ASA results, and thus the FS of $Fe_{1.063}Te$ shown in Fig. 3(b) of Ref. [1] is not correct. In addition, Fig. 3 of Ref. [1] does not show the FS in the a-b plane but it rather gives the top view (slightly tilted towards top right) of the full FS, and in the caption, the positions of the Γ and M points have been interchanged.

We show in Fig. 1, the DOS and the FS of $Fe_{1+x}Te$ alloys calculated with the FP-LMTO and the KKR-ASA methods using the RBA, and with the KKR-ASA CPA method. For $x = 0$, our results are in agreement [3] with that of Refs. [1,4], which confirms the reliability of the ASA in the present context. For going from FeTe to $Fe_{1.068}Te$ using the RBA, we need to accommodate 0.544 excess electrons per Fe atom, requiring an upward shift in the FP-LMTO (KKR-ASA) Fermi energy, E_F, of ~0.39 (~0.38) eV. Similarly, the shift for $Fe_{1.141}Te$ is found to be ~0.68 (0.67) eV. Within the RBA, our FP-LMTO and KKR-ASA results are in good agreement with each other. However, Han and Savrasov find a shift of ~0.76 eV, almost twice as much as we do, for $Fe_{1.063}Te$. Note that their shift is close to our shift for $Fe_{1.141}Te$. As a result, the FS of $Fe_{1.063}Te$ as shown in Fig. 3(b) of Ref. [1] is not consistent with the RBA. Our FP-LMTO and KKR-ASA results for the FS of $Fe_{1+x}Te$ alloys, using the RBA, are shown in Figs. 1(a) and 1(b), and for $x = 0$, they are in agreement with Refs. [1,4]. Not surprisingly, Fig. 3(b) of Ref. [1] is closer to the FS of $Fe_{1.141}Te$ as shown in our Fig. 1(a).

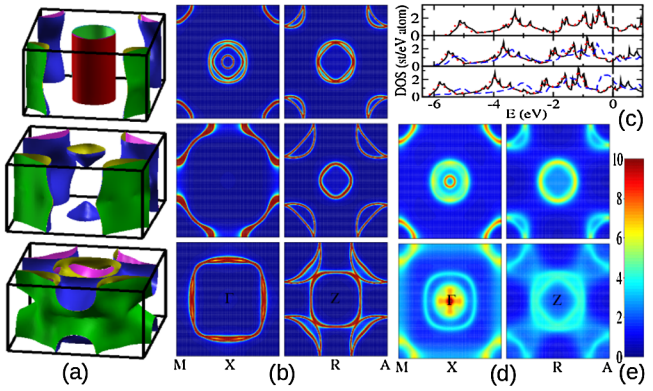

FIG. 1 (color online). (a) The Fermi surface of FeTe (top), $Fe_{1.068}Te$ (middle) and $Fe_{1.141}Te$ (bottom) using FP-LMTO method and the RBA. In FeTe, there is a small, closed cylinder-like structure at the center, which is not visible. (b) The FS of FeTe (top), $Fe_{1.068}Te$ (middle) and $Fe_{1.141}Te$ (bottom) in Γ-X-M and Z-R-A planes, calculated with KKR-ASA in the RBA. (c) The DOS of FeTe (top), $Fe_{1.068}Te$ (middle), and $Fe_{1.141}Te$ (bottom) obtained using FP-LMTO (black, solid line) and KKR-ASA (red, dotted line) within the RBA. The CPA DOS (blue, dashed line) for $Fe_{1.068}Te$ and $Fe_{1.141}Te$ are also shown. (d) The FS of $Fe_{1.068}Te$ (top) and $Fe_{1.141}Te$ (bottom), calculated with KKR-ASA CPA method. (e) The color map used in (b) and (d).

We find the KKR-ASA CPA DOS of $Fe_{1.068}Te$ and $Fe_{1.141}Te$, shown in Fig. 1(c), to be very different from the rigid-band results of both the FP-LMTO and the KKR-ASA methods. The CPA DOS moves up and there is a substantial redistribution of states throughout the energy range, especially around E_F, making the RBA quite inaccurate. The inadequacies of the RBA are further revealed by comparing the CPA FS, shown in Fig. 1(d) with that of the rigid band. The diffused intensity in Fig. 1(d) indicates the effects of disordering due to excess Fe in FeTe alloys.

Prabhakar P. Singh
Department of Physics
Indian Institute of Technology Bombay
Powai, Mumbai- 400076, India

Received 19 October 2009; published 4 March 2010
DOI: 10.1103/PhysRevLett.104.099701
PACS numbers: 74.70.−b, 71.18.+y, 71.20.−b, 75.25.−j

[1] M. J. Han and S. Y. Savrasov, Phys. Rev. Lett. **103**, 067001 (2009).
[2] P. P. Singh, arXiv:0908:0303.
[3] See supplementary material at http://link.aps.org/supplemental/10.1103/PhysRevLett.104.099701.
[4] A. Subedi, L. Zhang, D. J. Singh, and M. H. Du, Phys. Rev. B **78**, 134514 (2008).

