Reply to Comment on "Nonmagnetic Impurity Resonances as a Signature of Sign-Reversal Pairing in FeAs-based Superconductors"

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In Ref. [1], starting from two Fe ions per unit cell and two degenerate orbitals per Fe ion, I have constructed a two-orbital four-band tight-binding model, which describes correctly the characteristics of the Fermi surfaces in the FeAs-based superconductors. Most recently, based on this model, we have investigated antiferromagnetism and superconductivity in electron-doped samples by employing Bogoliubov-de Gennes equation [2]. It is shown that the coherence peak at positive bias energy is lower than that at negative energy for over-doped samples while the coherence peak at positive energy becomes higher due to the coexistence of spin density wave and superconductivity for under-doped samples. Meanwhile, the heights of the coherence peaks at negative and positive bias energies are approximately equal for overdoped samples. The results are consistent with recent scanning tunneling microscopy (STM) observations [3]. To the best of my knowledge, no other models can fit all the features of local density of states (LDOS) up to now.

In the preceding Comment [4], Daghofer and Moreo pointed out that the energy band structure in Ref. [1] is not degenerate at Γ point, which is contradictory to local density approximation or a Slater-Koster approach. Here I emphasize that the two-orbital four-band tight-binding model in Ref. [1] is built to fit angle resolved photoemission spectroscopy (ARPES) experiments rather than other theoretical calculations. The authors of this Comment seem to miss the important ARPES observations in over-doped samples, where the ω band disappears, but the β band still exists (see Fig. 3 in Ref. [5] and Figs. 3 and 4 in Ref. [6]). Therefore, it is obvious that the local density approximation or Slater-Koster approach is inconsistent with the experimental facts near Γ point. The disappearance of ω band leads to the asymmetric coherence peaks in LDOS [2], which were also observed by the STM experiments [7,8].

The authors of this Comment also argued that t2 and t3 in Ref. [1] are equal due to the symmetric hopping paths. However, this is only their opinion. It is known that the FeAs-based superconductors are very complex materials due to electron or hole doping, magnetic moment on Fe ion, and lattice distortions. In inelastic neutron scattering experiments [9,10], the magnetic excitation structure exhibits strong C2 (180◦) symmetry such that the nearest neighbor exchange constants along a and b axes are dramatically different due to tiny lattice distortions.

In Ref. [11], Nascimento et al. found different Fe-As orbital structure associated with distinct As ions. In recent STM experiments [12], Chuang et al. have also observed the local electron states with C2 rather than C4 (90◦) symmetry. This local electron property is not produced merely due to crystal symmetry [12]. The inequality of t2 and t3 could reflect these experimental facts. The difference of t2 and t3 determines the sizes of hole pocket around the Γ point and electron pocket around the M point, depending on the samples studied.

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