Influence of Co and Ni Doping on the Electronic Structure of $FeTe_{0.65}Se_{0.35}$

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Abstract: Despite the passage of more than 10 years since the discovery of unconventional superconductivity in iron compounds, the explanation of the occurrence of this phenomenon remains one of the most important tasks of solid state physics. Doping of these materials with transition metals can lead, depending on the system, to induction or suppression of superconductivity. Examination of the phase diagrams obtained in this way is one of the most important methods used in attempts to understand these compounds. Systematic investigations of electronic structure were performed for Co and Ni substituted FeTe0.65Se0.35 superconductor by means of angle-resolved photoemission spectroscopy (ARPES) and DFT calculations. Three hole pockets at the Γ point and one electron pocket at the M point were observed and the values of the band shifts near M and Γ point were estimated. The measurements revealed the rigid band model like shift of the band structure caused by the electron doping. It was found that one of the bands changes shape from almost linear to parabolic, when crossing Fermi level, which is result of strong correlations in the system. Comparison between experiment and DFT calculations allowed to determine mass renormalization. The data indicate that doping increases the electron pockets volume at the Fermi surface however, volume of the experimental Fermi surface is much smaller than predicted from calculations. The shape of the pockets near the M point changes significantly for highly doped samples. A clear shift of the hole pocket below the Fermi energy, which is observed in Co and Ni doped systems, indicate that the Lifshitz transition is realized in these systems.

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