

Abstract Submitted
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Localization Effects of Cu Substitutions in FeSe: an Improved Green's Function Decoupling Approach¹ YANG LIU, YUN SONG, Department of Physics, Beijing Normal University — We study the substitution effects of Cu in FeSe system by using a Green's function decoupling method based on an extended Hubbard-I approximation. A three-band Hubbard Hamiltonian with randomly distributed impurities is employed to describe the iron superconductor $\text{Fe}_{1-x}\text{Cu}_x\text{Se}$. The parameters of the three-band model are determined by fitting the Fermi structures with the results of experiments. With the increasing of Cu substitution, the nesting between hole-like and electron-like Fermi pockets is destroyed completely. We also find that Cu substitution can introduce strong localization effects and lead the system to have a metal- insulator transition.

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Yang Liu
Department of Physics, Beijing Normal University

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