

Abstract Submitted
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Do Transition Metal Substitutions Dope Carriers in Iron Based Superconductors?¹ TOM BERLIJN, Brookhaven National Laboratory, CHAI-HUI LIN, Stony Brook University, WEI KU, Brookhaven National Laboratory — We investigate the currently debated issue concerning whether transition metal substitutions dope carriers in iron based superconductors. From first-principles calculations of the configuration-averaged spectral function [1,2] of BaFe_2As_2 with disordered Co/Zn substitutions of Fe, important doping effects are found beyond merely changing the carrier density. While the chemical potential shifts suggest doping of a large amount of carriers, a reduction of the coherent carrier density was found due to the loss of spectral weight. Therefore, none of the change in the Fermi surface, density of states, or charge distribution can be solely used for counting doped coherent carriers, let alone presenting the full effects of the disordered substitutions. Our study highlights the necessity of including disorder effects in the studies of doped materials in general. [1] W. Ku, T. Berlijn, and C.-C. Lee, Phys. Rev. Lett. 104, 216401 (2010) [2] T. Berlijn, D. Volja and W. Ku, Phys. Rev. Lett. 106, 077005 (2011)

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