

Abstract Submitted
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Effects of single- and multi-substituted Zn ions in doped-122 type iron-based superconductors YUANYUAN ZHAO, BO LI, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas 77204, USA, WEI LI, State Key Laboratory of Functional Materials for Informatics and Shanghai Center for Superconductivity, Shanghai Institute of Microsystem and Informat, HONG-YI CHEN, National Taiwan Normal University, Department of Physics, Taipei 116, Taiwan, KEVIN E. BASSLER, C. S. TING, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas 77204, USA — Recent experiments on Zn-substituted 122-type iron-based superconductors at electron- and hole-doped region provide us with a testing ground to understand the effect of Zn impurities in the system. Here, our first-principle calculations of the electronic structure reveal the Zn 4s-orbital is partially occupied, suggesting the effect of Zn 4s-orbital could not be neglected. We focus on Zn 4s-orbital instead of its 3d-orbital. Through self-consistent lattice Bogoliubov-de Gennes (BdG) calculation on a two-orbital model, our results qualitatively agree with the experimental measurements.

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