

Abstract Submitted
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Correlation induced self-doping in the iron-pnictide superconductor Ba₂Ti₂Fe₂As₄O J.Z. MA¹, P. RICHARD, G.F. CHEN, H. MIAO, L.K. ZENG, Institute of Physics, Chinese Academy of Sciences, A.VAN ROEKEGHEM, S. BIERMANN, Centre de Physique Thorique, Ecole Polytechnique, N. XU, M. SHI, Paul Scherrer Institute, Swiss Light Source, Z.H. LIU, J.B. HE, S.C. WANG, Department of Physics, Renmin University, C. CAO, Department of Physics, Hangzhou Normal University, Y.L. SUN, G.H. CAO, Department of Physics, Zhejiang University, T. QIAN, H. DING, Institute of Physics, Chinese Academy of Sciences — The electronic structure of the intercalated iron-based superconductor Ba₂Ti₂Fe₂As₄O (T_c ~ 21.5 K) has been investigated by using ARPES and combined LDA + DMFT calculations. The electronic states near the Fermi level are dominated by both the Fe 3d and Ti 3d orbitals, indicating that the spacing layers separating different FeAs layers are also metallic. By counting the enclosed volumes of the Fermi surface sheets, we observe a large self-doping effect, i.e., 0.25 electrons per unit cell are transferred from the FeAs layer to the Ti₂As₂O layer, leaving the FeAs layer in a hole-doped state, which is in contrast with the LDA prediction of an electron-doped FeAs layer. This exotic behavior is successfully reproduced by the LDA + DMFT calculations, in which the self-doping effect is attributed to the electronic correlations in the Fe 3d shell. Our work provides an alternative route of effective doping without element substitution for iron-based superconductors.

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