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Of substitution and doping: Spatial and electronic structure in iron pnictides S. SCHUPPLER, P. SCHWEISS, P. NAGEL, M.-J. HUANG, R. EDER, TH. WOLF, H. V. LÖHNEYSEN, M. MERZ, Karlsruhe Institute of Technology (KIT) — A highly intriguing aspect in iron-pnictide superconductors is the composition-dependent electronic structure, in particular the question if and how charge carriers are introduced to the system upon substitution of Ba by alkali metals or of Fe by other transition metals, TM. We report on a systematic study of spatial structure and electronic states by x-ray diffraction and x-ray absorption, performed on a large number of compositions in the $(Ba,K)(Fe,TM)_2As_2$ family of compounds. The coherent combination of detailed structural information with an in-depth analysis of the electronic structure allows us to disentangle very sensitively "doping" effects from "substitutional" effects. This balance between substitution and doping turns out to be crucial for an understanding of magnetism and superconductivity in iron pnictides.

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