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Substitution and “site-decoupled doping” in iron pnictides M. MERZ, P. SCHWEISS, P. NAGEL, M.-J. HUANG, A. PLOG, R. EDER, TH. WOLF, H. V. LÖHNEYSSEN, S. SCHUPPLER, Karlsruhe Institute of Technology, Germany — The composition-dependent electronic structure of iron pnictides, in particular the question if and how charge carriers are introduced to the system upon substitution – by Sr or alkali metals, *AM*, for Ba; by transition metals, *TM*, for Fe; and/or by P for As – continues to provide surprises. Our ongoing 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 $(\text{Ba,Sr},AM)(\text{Fe},TM)_2(\text{As,P})_2$ family of compounds, shows, for instance, that valences are rarely as expected, that doping can be “effective” or “slow” depending on substituent, and that most doping effects are completely “site decoupled”, meaning that they occur *either* on the Fe site *or* on the As site but not on both simultaneously. Furthermore, the energy-level schemes derived from electronic and spatial structure differ from the present “standard” assumptions. In all, it appears that substitutional effects may be more crucial to magnetism and superconductivity in iron pnictides than direct doping effects.

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