Orbital and charge ordering in the $RE_{1-x}Ca_xTiO_3$

A. C. Komarek[1,2], C. Schüßler-Langeheine[1], H.-H. Wu[1], M. Reuther[1], N. Hollmann[1], T. Lorenz[1], A. Cousson[3], F. Bourée[3], P. Link[2], D. Trots[4], C. Baeths[4], W. Morgenroth[4], R. Feyerherm[5] and M. Braden[1]

1: II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln
2: Technische Universität München, FRM-II, D-85747 Garching
3: Laboratoire Leon Brillouin, CEA-CNRS, CE-Saclay, F-91191 Gif-sur-Yvette
4: Hasylab/DESY, D-22607 Hamburg
5: HMI at BESSY, Albert Einstein Str. 15, D-12489 Berlin

Keywords: charge ordering, metal-insulator transition, neutron scattering

With a single electron in the 3d shell, the rare-earth (*RE*) titanates $RETiO_3$ have attracted strong interest for studying the complex interplay of charge, orbital and magnetic degrees of freedom. Substituting a divalent earth-alkali for the *RE*, a metal-insulator transition is induced, which in case of $La_{1-x}Sr_xTiO_3$ occurs at a few percent whereas $Y_{1-x}Ca_xTiO_3$ stays insulating up to rather high doping. We studied the hole-doped systems $(Y,Er,Lu)_{1-x}Ca_xTiO_3$ by various diffraction techniques, by resistivity and by magnetic susceptibility measurements. These systems show a complex phase diagram of structural distortions accompanying the metal-insulator transition. There is coexistence of an insulating monoclinic phase with a metallic low-temperature orthorhombic phase. Our neutron and resonant x-ray diffraction data unambigously prove that charge ordering occurs in the monoclinic phase. Even away from half-doping, we find two distinct Ti sites in a checkerboard arrangement. This charge ordering allows one to explain the persistence of the insulating states up to high doping.