Pressure-driven structural distortion and band gap closure in transition-metal perovskites

LOA I.[1], SYASSEN K.[1], WANG X.[1], ROTH H.[2], and LORENZ T.[2]
[1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany
[2]Universität zu Köln, II. Physikalisches Institut, D-50937 Köln, Germany

Orbital ordering, fluctuation, and excitation phenomena in transition metal perovskites have been investigated in recent years both experimentally and theoretically. In this context, rare-earth titanates with three nearly degenerate $3d(t_{2g})$ orbitals, which are occupied by a single electron, have been of particular interest. We address here the question of how robust the orbital ordering is in $YTiO_3$, and show that it may possibly be tuned by the application of hydrostatic pressure. By means of synchrotron x-ray powder diffraction we investigated structural details of $YTiO_3$ up to 30 GPa. Marked changes in the distortion of the TiO_6 octahedra were observed at around 10 GPa, indicating the possibility of an orbital reorientation. In addition to the structural aspects, we have studied the pressure-induced charge delocalization and metallization in $YTiO_3$ and other perovskites by synchrotron infrared micro-spectroscopy in the mid- and far-infrared spectral ranges. The optical band gap shifts in $YTiO_3$ and $LaMnO_3$ under pressure were determined quantitatively. The combined results on the structural, orbital and electronic changes under pressure give new insight into the physics of these materials.

This work was performed in collaboration with Y.-L. Mathis, B. Gasharova, and D. Moss (ANKA, Karlsruhe, Germany); M. Amboage and M. Hanfland (ESRF, Grenoble, France); O. K. Mel'nikov and A. Ya. Shapiro (Russian Academy of Science, Moscow, Russia).