Pressure-Driven Orbital Reorientation and Band Gap Closure in Transition-Metal Perovskites

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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 3*d*(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 can be tuned by the application of hydrostatic pressure. By means of synchrotron x-ray powder diffraction we investigated the crystal structure of $YTiO_3$ up to 30 GPa. The evolution of the distortion of the TiO_6 octahedra indicates a pressure-driven spatial reorientation of the t_{2g} wavefunction at around 10 GPa. We will discuss this observation in comparison with experimental results on the related compounds $LaTiO_3$ and $LaMnO_3$. In addition to the structural aspects, we have investigated the pressure-induced charge delocalization and metallization in these three perovskites by synchrotron infrared micro-spectroscopy in the mid- and far-infrared spectral ranges. The optical band gap shift in $YTiO_3$ and $LaMnO_3$ under pressure was determined quantitatively. The combined results on the structural, orbital and electronic changes under pressure give new insight into the physics of these materials.

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