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Synchrotron electron density - property relationship for metal oxides

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The relationship of the one-electron density to the optical and magnetic properties for metal oxides was studied by imaging the deformation electron density (DD) with synchrotron x-radiation. The high accuracy of DD images at the Photon Factory in Japan allows the reorganization of the electron density in the atoms that form crystalline solids to be depicted unambiguously, sometimes with surprising conclusions.

For the birefringent carbonates, $MaCO_3$ (Me=Ca, Mg, Mn), the DD correlates with optical anisotropy to a degree consistent with a cause and effect relationship between electron density and refractive index. That index is large, where locally antisymmetric components are strong, and small for directions such that locally symmetric components in the density dominate.

The synchrotron DD images for $MeMe'O_3$ oxides with corundum structure (Me=Me'=Al or Fe), with C-type structure (Me=Me'=Rare Earth) and with perovskite structure (Me=Rare Earth and Me'=Fe) depict higher DED local symmetry around metals, which becomes progressively more pronounced for the heavier magnetic cations. Electron density of overlapping cations' closed inner subshells is repelled by exchange towards regions of lower electrostatic potential more remote from the nuclei. The transferred density retains the cation's symmetry. These metal-metal interactions are beyond the normal range of chemical bonds. When spin-dependent, they must play important roles in magnetic ordering and in structural transitions.