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XANES studies of the Lithium Molybdenum Purple Bronze $Li_{0.9}Mo_6O_{17}$

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ABSTRACT

X-ray absorption near-edge spectroscopy(XANES) was performed to investigate the electronic structure of transition-metal oxides. Mo $L_{3,2}$ and O K absorption edges for pure Mo, MoO_2, MoO_3, and $Li_{0.9}Mo_6O_{17}$ were measured.

The lithium molybdenum purple bronze has a three-dimensional crystal structure(one-third of the molybdenum atoms are located in oxygen tetrahedra, while the others are within oxygen octahedra), but it exhibits pseudo-one-dimensional metallic character, eventually becoming a super conductor at ~2 K after the anomalous upturn of the resistivity at about 25 K with decreasing temperature.

O K edges(1s → p transition) might be reflected to some extent the d-density of states around the metal atoms, because in a molecular-orbit picture the d-orbitals of the metal atoms mix with the p-orbital from the oxygen atoms. We discuss to clarify the d-states for the molybdenum oxides by comparison of both the Mo $L_{2,3}$ and O K edges.

The observed increases of white-line feature strength at the O K and L_3 edges indicate that the local density of unoccupied 4d states decline with increasing the number of oxide. These differences are interpreted on the basis of structural difference with the number of oxides.

By predictions from ligand-field theory, we can find crystal structure using both the splitting and the relative intensities of the white-line features. For MoO_3 the more intense component of the split 2p → 4d transition is at lower energy, while for MoO_2 it is at higher energy. Our experimental results supports the crystal structure of $Li_{0.9}Mo_6O_{17}$ [M.Onoda etal, J. Sol. State Chem. 66, 163 (1987)]

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