Electronic Structure and Metal-insulator Transition of $Ca_{2-x}Sr_xRuO_4$ Studied by NEXAFS

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Introduction: Sr_2RuO_4 is still the only superconductor that is isostructural to a high-temperature superconductor but does not contain copper. Its superconducting and magnetic properties are unconventional [1,2], and with three Ru-O derived bands crossing E_F it exhibits a rich electronic structure [1,3,4]. Substituting Sr by Ca leads to distortions of the crystal structure and to a (Mott-type?) metal-insulator transition at $x \approx 0.2$; for Ca-rich samples antiferromagnetic ordering becomes possible [5].

Methods and Materials: With polarization-dependent NEXAFS at the O 1*s* absorption edge we investigated the unoccupied electronic structure for a series of $Ca_{2-x}Sr_xRuO_4$ single crystals, with emphasis on samples near the metal-insulator transition. Bulk-sensitive fluorescence detection was employed.

Results and Conclusions: Compared to pure Sr_2RuO_4 (cf. [3]) the main spectral features change moderately with Ca content; a more detailed analysis is facilitated by fitting with asymmetric Gaussians. The changes of peak positions with *x* reflect well the symmetry changes of the RuO_6 octahedra, while the development of the spectral weight of the various features points to charge carrier redistribution near E_F as well as to changes in bandwidths and hybridization strengths due to the structural distortions. The most intriguing aspect of this study is the clear Hubbard-like splitting of a near-E_F feature that becomes stronger with increasing Ca content: although the Hubbard correlation energy *U* for Ru is not very large in itself, it is very close in value to the bandwidths of two near-E_F bands [1] – and in turn our NEXAFS observation of the Ca-induced splitting directly shows the increased importance of correlation effects due to band narrowing for the Ca-rich compounds.

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