Half-metallic ferromagnetic transition metal oxides: Correlated electronic structure of bulk CrO_2 from hard X-ray photoemission

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CrO_2 has theoretically been predicted to be a half-metallic ferromagnet [1], i.e. a metal for one spin component and an insulator for the other one. The motivation for the recent very intense experimental investigations of this material has been its potential use as spin injector in spintronics for, e.g., tunnel magnetoresistance [2] and spin-momentum transfer torque switching of magnetizations [3]. The original experimental test of the electronic structure by spin- and angle-resolved photoelectron spectroscopy (SPAR-PES) [4] using a photon energy of hν = 21.2 eV (i.e. small photoelectron escape depth) yielded a spin polarization of 90%, but not a well pronounced Fermi edge. It was conjectured whether the material is closer to a Mott insulator rather than a metal obeying a $\rho \sim T^2$ law [5]. Hence, there is an ultimate need about getting experimental information of the bulk electronic structure of CrO_2 , like for many other oxide materials [6].

We present the first comprehensive investigation of electronic core states and valence band states of CrO_2 by means of hard X-ray photoelectron spectroscopy (HAX-PES) using photon energies of hν ~ 8 keV [7]. The use of HAXPES with a relatively large photoelectron escape depth yields a first real bulk-sensitive investigation of the electronic structure of CrO_2. However, while we observe a pronounced metal-type Fermi edge for hν = 700 eV, it is almost absent in HAX-PES. This fact is attributed to a recoil effect of the photoelectrons, shifting spectral weight from near E_F to below it. In addition, a well screened feature is found in the Cr $2p_{3/2}$ core level, consistent with the metallicity of CrO_2. The lower and upper Hubbard band could be identified by HAX-PES and inverse PES, respectively, resulting in an experimental value of Hubbard U ~ 3.5 eV, which is in good agreement with U = 3.0 eV in LSDA + U calculations.[8] In HAX-PES the intensity near E_F is rather small, but finite and temperature independent. This excludes an enhanced density of states at E_F as conjectured in the framework of an orbital Kondo effect using LDA + DMFT calculations.[9] –

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