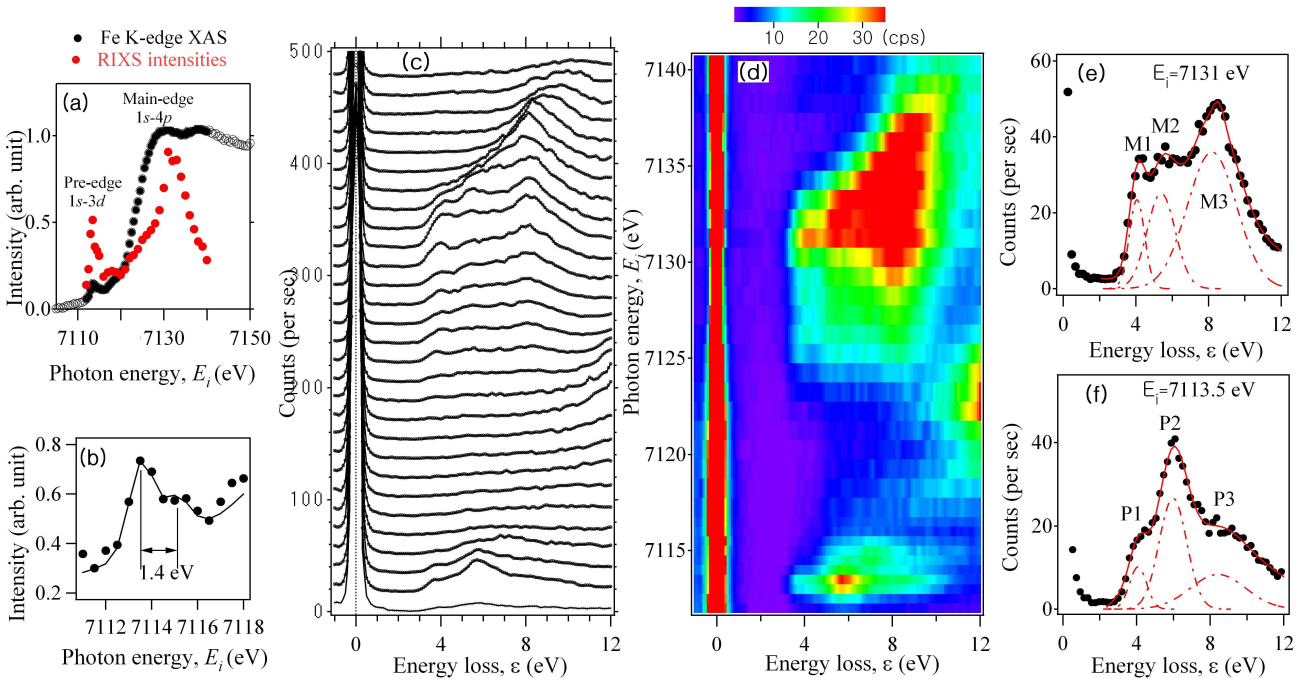

FIG. 2: (a) Fe K edge x-ray absorption spectrum (XAS) of $FeBO_3$ measured in PFY mode (black open dots) and integrated intensities of the RIXS spectra of (c) (red filled dots). (b) XAS same as in (a) but shown on the expanded scale of E_i around the pre-edge. (c) RIXS spectra measured for different incident photon energies 7112 eV $\leq E_i \leq$ 7140 eV. (d) 2D plot of the RIXS spectra of (c). (e) and (f) show representative RIXS spectra of the main-edge RIXS (E_i=7131 eV, Q=(0 0 9)) and the pre-edge RIXS (E_i=7113.5 eV, Q=(0 0 9)), respectively. Gaussian functions are used to fit inelastic peaks, while the Voigot function is used to fit the elastic line (see the text).

function of the excitation energy, momentum transfer, polarization, and temperature. We show that unlike previously studied cases, the K edge RIXS can probe both CT and MH excitations at the same time. We interpret the pre-edge and the main-edge RIXS excitations as MH and CT excitations, respectively, and derive important quantities including the charge-transfer gap Δ_G and the Mott-Hubbard gap U_G using molecular orbitals (MO) in the cluster model and multiplet calculation in the many-electron multiband model. This study demonstrates a special quality of the K edge RIXS to be a simultaneous probe of CT and MH excitations in TM compounds.

II. EXPERIMENT AND SAMPLE

The RIXS measurements were performed using the MERIX spectrometer at the XOR-IXS 30-ID beamline of the Advanced Photon Source (APS). The sample is mounted in the Displex closed-cycle cryostat NE-202N with a temperature range of 6 K to 450 K. The measurements were carried out at room temperature and at temperatures close to the Neél temperature (T_N=348 K). X-rays impinging upon the sample were monochromatized to a bandwith of 75 meV, using a four-bounce (+ − −+) monochromator with asymmetrically cut Si(400) crystals.[30] The beam size on the crystal was reduced to 45(H)×20(V) μm^2 by focusing in the Kirkpatrick-Baez configuration. The photon flux on the sample was 1.1×10^{12} ph/s. The total energy resolution of the MERIX spectrometer at the Fe K edge is 180 meV. This is achieved using a Ge(620) spherical diced analyzer, and a position-sensitive microstrip detector placed on a Rowland circle with a 1 m radius. The silicon microstrip detector with 125 μm pitch is applied for the purpose of reducing the geometrical broadening of the spectral resolution function.[31] Maximum RIXS count rates were in the range of 40-50 Hz. Horizontal scattering geometry, where the incident photon polarization vector component is parallel to the scattering plane (π-polarization), was used for all RIXS measurements, with the crystal **c**-axis in the scattering plane as shown in Fig. 1(a).

Iron borate, $FeBO_3$, single crystal with low-dislocation density, grown by spontaneous crystallization from flux,[32] was used in the current experiment. The crystal has a form of a platelet $6 \times 7 \times 0.15$ mm^3, with **c**-axis perpendicular to the platelet surface. Iron borate has a rhombohedral calcite structure that belongs to the space group $R\bar{3}c(D^6_{3d})$ with two formula units per unit cell. The lattice constants are **a**=**b**=4.626(1) $\AA$ and **c**=14.493(6) $\AA$. The Fe^{3+} ions are centered in a slightly distorted O^{2+}_6 octahedra. The octahedral O_h crystal field splits the energy of the 3d orbitals into three-fold degenerate t_{2g} and two-fold degenerate e_g states. As depicted