Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Theoretical analysis of high-resolution X-ray absorption spectra and 2p-3d resonant X-ray emission spectra of CeO_2 HIRONORI TONAI, Osaka Prefecture University, NAOMI KAWAMURA, MASAICHIRO MIZUMAKI, JASRI/SPring-8, TAKAYUKI UOZUMI, Osaka Prefecture University — The $3d$ and $4f$ systems show various attractive phenomena due to strong electron correlations. The X-ray core-level spectroscopy, such as X-ray absorption spectroscopy (XAS), is an efficient technique to investigate electronic states of the systems. Recent years, the experimental techniques have been rapidly developing, and, especially, the progress in the experimental resolution has enabled us to observe fine spectral features. For example, a pioneering work was made by K. Hmlinen et al.[1] Recently, we performed high-resolution XAS experiments (partial fluorescence yield; PFY) and observed a peak corresponding to $2p$-$4f$quadrupole transition around the pre-edge region of the L_3-edge of CeO_2. Conventionally, X-ray spectra have been analyzed using a phenomenological impurity Anderson model (IAM). However, such a simplified model does not seem to appropriate for analysis of high-resolution spectrum because of possible ambiguities from the choice of adjustable parameters included. Thus we constructed an IAM framework combined with a first principle band calculation. In this meeting, we report experimental results and theoretical analysis for the PFY spectrum and $2p$-$3d$ resonant X-ray emission spectroscopy. [1] K. Hmlinen et al., PRL 67 (1991) 2850.

Hironori Tonai
Osaka Prefecture University

Date submitted: 06 Nov 2015 Electronic form version 1.4