Theoretical study of $L_{2,3}$ edge X-ray absorption spectra of vanadium oxide and chromium oxide using multichannel multiple scattering method

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X-ray absorption spectroscopy is used as a method to investigate the structure and electronic state of materials. Especially, $L_{2,3}$ edge is useful to investigate fine structure of electronic state. However, theoretical analysis was difficult due to the influence of the spin-orbit interaction of the 2p orbital and the Coulomb interaction caused by the overlap of the photoelectron and core electron wave functions. By applying the multi-channel (MC) multiple scattering theory incorporating this interaction to highly symmetric metal oxide, it has been reported that the spectrum is improved compared to the conventional independent particle calculation [1]. The purpose of this study is to apply MC theory to V_2O_5 and CrO_3, which have low symmetry, to verify the validity of the theory and to analyze its spectrum.

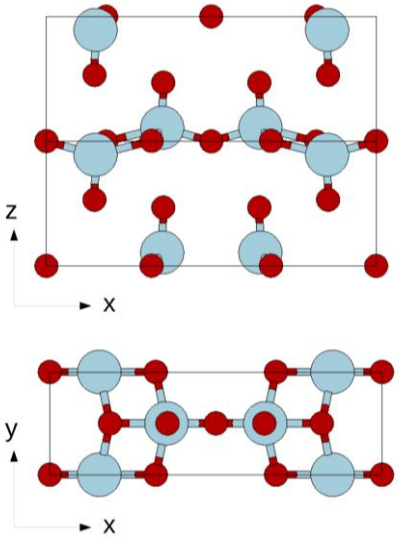

Figure 1 Structure of V_2O_5. Red is oxygen, blue is vanadium.

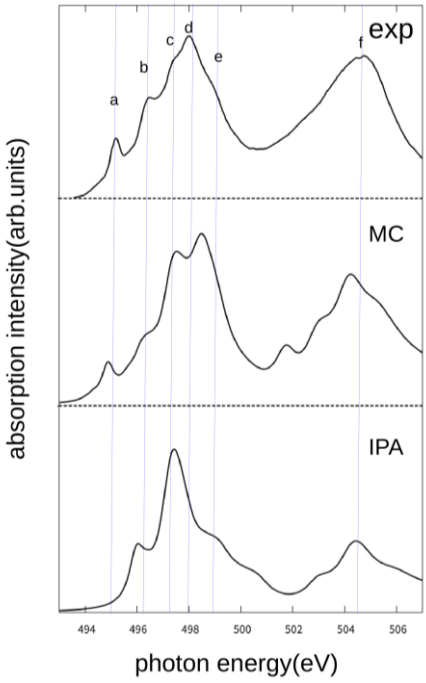

Figure 2 X-ray absorption spectra of $L_{2,3}$ edge of V_2O_5. Top: experiment [2]. Middle: multichannel (MC). Bottom: independent particle (IPA)

Reference

[1] P. Krüger Phys. Rev. B 81, 125121 (2010)

[2] D. Maganas et al., Phys. Chem. Chem. Phys. 15, 7260 (2013)