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Distortions in 2p4d Partial Fluorescence yield for 4d elements[1]
ALEXANDER PRICE, Georgia Regents University, FRANK DE GROOT, Utrecht University, TRINANJAN DATTA, Georgia Regents University — X-ray absorption spectroscopy (XAS) is a standard tool to determine the electronic structure of molecules and materials. CTM4XAS and CTM4RIXS are semi-empirical programs to analyze transition metal L− and M− edge transitions by evaluating the effects of crystal field and charge transfer parameters on the atomic multiplets. We compute and compare the XAS and the fluorescence yield (FY) XAS, of the 3d and 4d transition metal ions. In the case of 2p edges of 3d elements Auger decay dominates and sets the time scale. The 2p3d X−ray emission spectra (XES) accounts for approximately 80% of the radiative decay. The 2p3d partial FY is distorted and because it dominates the FY, the total FY is also distorted. For the 4d elements the 2p4d XES decay is approximately 10% of 2p3d XES decay, implying that (the energy-constant) core-core XES and Auger channels dominate the decay. The computed 2p4d partial FY−XAS spectra are different from the 2p XAS. Although 2p4d partial FY is distorted, the total FY is not because it is dominated by 2p3d XES. We also find that the 2p3s and 2p4s XES channels contribute less than 1% and can be neglected.

[1]Cottrell Research Corporation

Alexander Price
Georgia Regents University

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