POSTER PRESENTATION

A MACHINE LEARNING APPROACH APPLIED TO DETERMINE FORMAL OXIDATION STATE OF 3D COMPOUNDS

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X-ray-absorption K-edge shifts of manganese, cobalt, and copper have been measured in different reference compounds at different structures and in different synchrotron beamlines in order to see if is possible using this edge shifts and machine learning methods to obtain information on the oxidation state of an unknown compound. In all cases, the shifts are the same sign, a fact that points to the absence of a significant uncompensated charge transfer from one elemental constituent to another. Identifying the edge shifts as core-level shifts, the Watson-Hudis-Perlman charge-compensation model is used on these systems, following the method proposed by Capehart et al [1]. We analyze the shift in energy from the pre-peak (taking E = 0; internal reference point) to fulfill a certain fixed area. Due to this method employ an internal reference point, it is independent on the beamline energy calibration. In our first results combining K-edge spectra of Mn, Co and Cu samples at LNLS, ALBA, ESRF and Spring-8, the energy shifts have similarities at the same formal oxidation state. The goal is to get a large number of K-edge spectra obtained from different light sources in order to propose a generalized statistical analysis that calculates the oxidation state of a sample with a certain confidence level using this methodology. This algorithm to calculates oxidation states in now tested with several spectra of references of 3d materials (from Ti-K to Zn-K) and is incorporated into a program that does the estimation independently on the light source and establish limits between which the method is reliable.

REFERENCES:

[1] T. W. Capehart, J. F. Herbst, R. K. Mishra, and F. E. Pinkerton, Phys. Rev. B 52, 7907 (1995).

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