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The valence electronic structure of zinc oxide powders as determined by X-ray emission spectroscopy: variation of electronic structure with particle size

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Abstract

The valence electronic structure of zinc oxide was characterized by X-ray emission spectroscopy (XES). The different features in the XE spectra were identified by comparison with UPS data recorded for an O-terminated ZnO($0\,0\,0\,\bar{1}$) single crystal and with the aid of ab initio quantum chemical calculations explicitly considering the presence of the core hole. For zinc oxide powder samples, the influence of the specific surface area on the XE spectra was investigated in a comparative study. The spectra of all powder samples were found to be dominated by bulk contributions, but surface contributions as indicated by significant deviations from the bulk spectra were detected for powders with very high specific surface areas corresponding to a mean particle size in the 10 nm range.

Keywords: X-ray emission spectroscopy; UPS; ZnO