

SXAS and SXES Studies of Self-assembled ZnO Nanorods

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Introduction: Zinc oxide represents an important basic material (II-VI semiconductor) due to its low cost, wide bandgap as well as its electrical, optoelectronic, and luminescent properties. ZnO is of great importance for fundamental research as well as relevant for various fields of industrial and high technological applications. A low threshold lasing action is observed in the low-dimensional ZnO nanowire arrays¹. The development of purpose-built materials², has enabled the controlled aqueous synthesis of metal oxide particulate thin films with well-defined morphology, particle size, texture, and orientation on various substrates. Indeed, ZnO material with well-defined and well-controlled morphology such as, for instance, three-dimensional array of anisotropic and highly oriented crystallites should contribute to reach enhanced fundamental knowledge of the relation between structure and properties as well as contributing to the development of improved devices.

Methods and Materials: Soft x-ray originates from an electron transition between a localized core state and a valence state. The most striking features of x-ray spectroscopic characterization are (1) the atomic and site selectivity due to transitions involving core levels, and (2) the orbital and symmetry selectivity by virtue of dipole selection rules and the use of polarized x-rays from synchrotron radiation sources. In order to probe the orbital character and symmetry as well as its contribution to the conduction band of the microrods, we have compared its XAS spectra to the prediction of an *ab-initio*, full-potential calculation of periodic crystal ZnO. The experiments were carried out on ZnO microrods consisting of monodisperse, anisotropic and highly oriented crystallites grown on a commercial transparent conducting glass substrate (TCO)

Results: Figure 1 shows the experimental XAS and XES spectra in comparison with the calculated partial DOS of the O 2*p* unoccupied valence states. All the absorption and emission features are reproduced by the calculation. The experimental and theoretical findings suggest a strong correlation between the electronic structure of crystalline ZnO nanorod arrays.

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References: [1] M. H. Huang et al., *Science* **292** (8), 1897 (2001); [2] L.Vayssieres et al., *Mater. Res. Soc. Symp. Proc. (Nanoparticulate Materials)* Vol. 704 (2002).

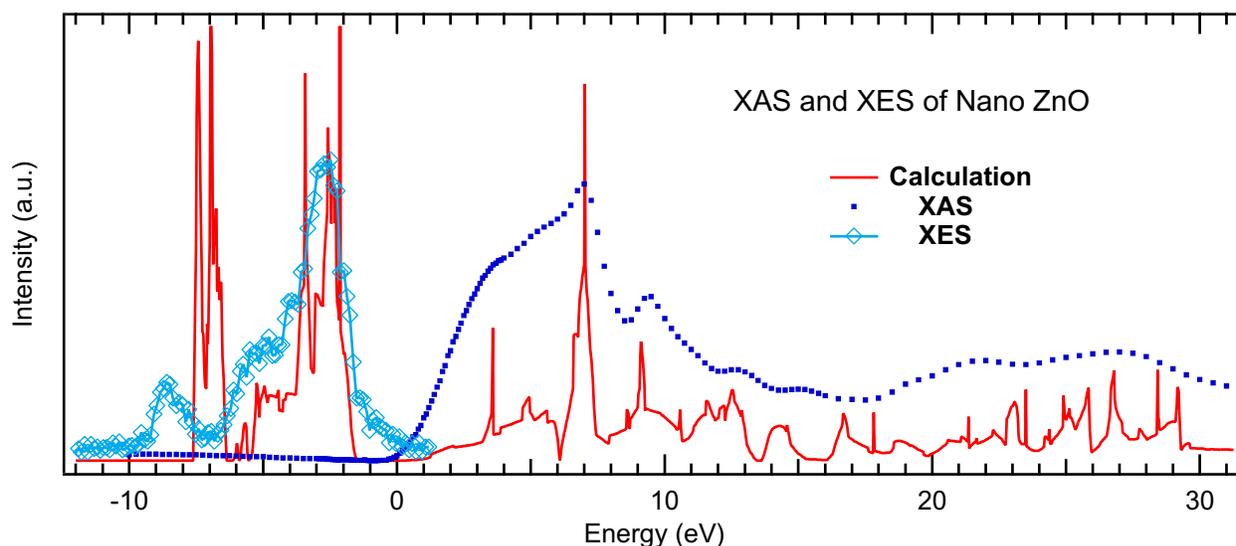


Figure 1. The experimental O 1s absorption spectrum (dotted line) and O K-emission spectrum (line and marks) of ZnO nanorods. The calculated oxygen 2*p* density of states (DOS) for ZnO crystalline.