Analyzing defect properties in oxides by x-ray photoelectron spectroscopy

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Defects and dopants are the key to understand and manipulate the properties of functional ceramics. Despite their importance, the knowledge about defect properties is mostly qualitative and based on separate concepts for the different possible charge compensation mechanisms. A combined quantitative treatment of the different charge compensation mechanisms is highly desirable and could pave the way for predicting material properties. Quantitative information on defect properties, such as their energy levels which determine the valence state, can directly be used for quantitative defect models but are still barely available from experiment. X-ray photoelectron spectroscopy (XPS) has the potential to fill this gap, as it provides simultaneous information on the valence states and on the position of the Fermi energy, which are intimately connected with each other. The technique is able to directly determine charge transition levels of dopants without any assumptions and model comparison and can be applied to doping concentrations even below 1%. As XPS is element specific, it can also be applied to materials in which more than a single dopant species is present. The presentation will give an overview on how defect properties can be analyzed with XPS. Experimental solutions for the challenge of measuring highly insulating samples will be demonstrated with examples from electronic, ionic and mixed ionic-electronic conductors and piezoelectric materials. The extend to which defect energy levels depend on concentration and the possibility to transfer defect energy levels between materials will be discussed. For some cases, the experimentally obtained defect properties will be compared with those calculated by means of density functional theory.