ADVANCED FUNCTIONAL MATERIALS

Zinc Oxide Nanoparticles with Defects**

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Dedicated to R. Kniep on the occasion of his 60th birthday

Zinc oxide in the form of nanoscale materials can be regarded as one of the most important semiconductor oxides at present. However, the question of how chemical defects influence the properties of nanoscale zinc oxide materials has seldom been addressed. In this paper, we report on the introduction of defects into nanoscale ZnO, their comprehensive analysis using a combination of techniques (powder X-ray diffraction (PXRD), X-ray absorption spectroscopy/extended X-ray absorption fine structure (XAS/EXAFS), electron paramagnetic resonance (EPR), magic-angle spinning nuclear magnetic resonance (MAS-NMR), Fourier-transform infrared (FTIR), UV-vis, and photoluminescence (PL) spectroscopies coupled with ab-initio calculations), and the investigation of correlations between the different types of defects. It is seen that defect-rich zinc oxide can be obtained under kinetically controlled conditions of ZnO formation. This is realized by the thermolysis of molecular, organometallic precursors in which ZnO is pre-organized on a molecular scale. It is seen that these precursors form ZnO at low temperatures far from thermodynamic equilibrium. The resulting nanocrystalline ZnO is rich in defects. Depending on conditions, ZnO of high microstructural strain, high content of oxygen vacancies, and particular content of heteroatom impurities can be obtained. It is shown how the mentioned defects influence the electronic properties of the semiconductor nanoparticles.