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Investigation of magnetic, morphological, structural, stability and optical properties of Ce3+ and Cu2+ co-doping in ZnO.

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Key words: Semiconductors, Electronic structure, Magnetic Properties, Optical properties Abstract: Ce3+, Cu2+ co-doped ZnO (Zn1_2xCexCux O: x¼0.00, 0.01, 0.02, 0.03, 0.04 and 0.05) nanocrystals were synthesized by the use of sol-gel technique. These nanocrystals were investigated by using X-ray diffraction (XRD), UV–visible diffuse reflectance spectroscopy (DRS), scanning electron microscopy (SEM), High-resolution transmission electron microscope (HR-TEM) and selected area electron diffraction (SAED). The stability and magnetic properties of Ce3+ and Cu2+ co-doped ZnO were probed by first principle calculations. XRD results revealed that all the compositions are single crystalline, hexagonal wurtzite structure. The optical band gap of pure ZnO was found to be 3.22 eV, which was in agreement with other experimental findings [1, 2] and it decreased from 3.22 to 3.10 eV with an increase in the concentration of Cu2+ and Ce3+ content. The morphologies of Ce3+ and Cu2+ co-doped ZnO samples confirmed the formation of nanocrystals with an average grain size ranging from 70 to 150 nm. The ab initio magnetization calculations results affirmed the antiferro and ferromagnetic state for Ce3+ and Cu2+ co-doped ZnO structure.

Reference: [1] J.F. Chang, W.C. Lin, M.H. Hon, Appl. Surf. Sci. 183 (2001) 18. [2] I. Djerdj, Z. Jaglicic, D. Arconde, M. Niederberger, Nanoscale 2 (2010) 1096.

Summary

Ce, Cuco-dopedZnOnanocrystals weresuccessfullysynthesizedbya microwavecombustionmethod. With Ce-Cu co-doping, crystallite size, latticeparametersandstrainof ZnO changes. The bandgapofthesynthesized samples hasbeenvariedintherange of 3.15-3.10eV. The grainsizeofthesampleisdecreased withtheincreaseinCe-Cu co-doping. The magnetizationmeasurements result intoferroandantiferromagnetic stateforallco-dopedsamples which isinagreementwith first principles theoreticalculations

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Prof. Dejene Birhanu Francis

DejeneBF@ufs.ac.za Department of Physics University of the Free State- Qwaqwa campus Private Bag X13 Phuthaditjhaba 9866 South Africa

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Primary author: Ms MULWA, WINFRED MUENI (UNIVERSITY OF THE FREE STATE PRIVATE BAG X13 PHUTHADITJHABA, 9866)

Co-author: Prof. DEJENE, FRANCIS BIRHANU (UNIVERSITY OF THE FREE STATE PRIVATE BAG X13 PHUTHADITJHABA, 9866)

Presenter: Ms MULWA, WINFRED MUENI (UNIVERSITY OF THE FREE STATE PRIVATE BAG X13 PHUTHA-DITJHABA, 9866)

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