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Authors: S. Sriram, K.C. Lalithambika, A. Thayumanavan

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## Experimental and theoretical investigations of photocatalytic activity of Cu doped ZnO nanoparticles

S.Sriram<sup>1\*</sup>, K.C. Lalithambika<sup>1</sup> and A.Thayumanavan<sup>1</sup>

*1. Department of Physics, School of Electrical & Electronics Engineering, SASTRA University, Thanjavur 613401. Tamilnadu, India.*

\*Corresponding Author:

S.Sriram  
Department of Physics,  
School of Electrical & Electronics Engineering,  
SASTRA University,  
Thanjavur 613401  
Tamilnadu India  
Email : [sukansriram@gmail.com](mailto:sukansriram@gmail.com)  
Phone + 91 9629020302

### Abstract:

Undoped and Cu doped ZnO nanopowders were synthesized by very simple and cost-effective soft chemical method by varying copper concentration as 10 at%, 20 at % and 30 at% for dye degradation test. Dense nanosheets of wurtzite structure with preferential growth of (101) were formed. The crystallite size decreases from 66.810 nm to 20.360 nm when the Cu content is increased. The photoluminescence results confirm the shift of near band edge emission (NBE) towards the lower wavelength with increasing doping concentration. Energy dispersive X-ray analysis (EDX) studies confirms the presence of Zn, O and Cu elements in the prepared nano powders. Photocatalytic activity test was conducted for the prepared nanopowders against Methylene Blue (MB) dye under visible light. The observed results show that the photocatalytic efficiency of the prepared nanopowders increase with the increase of Cu content. Theoretical study based on electrode potentials was performed by employing density functional theory (DFT) in order to validate the experimental results.

**Keywords:** ZnO nano powders; Cu doped ZnO; photocatalytic activity; DFT; Structural Studies;

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