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# Alteration of the electronic structure and the optical properties of graphitic carbon nitride by metal ion doping

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## Abstract

The photoluminescence quenching of graphitic carbon nitride (GCN) was systematically investigated with the doping of transition metal ions. The photoluminescence spectra of metal doped and pristine GCN were monitored and the trend of quenching efficiency was found to be  $\text{Cu}^{2+} > \text{Co}^{2+} > \text{Mn}^{2+}$ . Interestingly, with the increasing doping concentration of different metal ions simultaneous red shift and luminescence quenching was determined in the photoluminescence spectra as well as increased absorption tail in longer wavelength hence enhancement in the bandgap. The change in the optical properties could be mainly due to structural reconstruction and doping induced electronic redistribution is discussed.

**Keywords** : photoluminescence; optical properties; luminescence; energy; graphitic carbon nitride

## 1. Introduction

Recent progress in the development graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) materials has attracted severe attention due to its widespread applications [1] due to its high thermal and chemical stability, nontoxicity, facile to produce [2-8] and excellent optical property. The first of polymeric graphitic carbon nitride was synthesized by Berzelius and named by Liebig in 1834 [9] which emerges as a promising optoelectronic material for applications [11-18]. However, it suffers from inherent low conductivity and efficiency due to bandgap limitations and electron mobility. Numerous methods have been employed for effective utilization of efficiency of carbon nitride and its proper bandgap (2.7eV) [10] such as structural and modifications, cation and anion doping and composite heterostructures [19-29]. Among those, non-metal ion doping such as boron, sulphur, and fluorine doping into the carbon nitride lattice have been studied which shows the enhance visible light absorption, red shift in the absorption spectrum, narrowing the bandgap greatly improved the electronic and optical properties of g-C<sub>3</sub>N<sub>4</sub>. Although, there have been few reports on modification of carbon nitride structures, a metal doped carbon nitride study and their effect on optical, structural and electronic properties is still lacking. It is speculated that the incorporation of metal ions into the carbon nitride could alter the electronic structure and bandgap with tunable optical properties.

It is recognized that the conduction band and valence band can be reform by ion doped lattice modification which could significantly influence the surface properties and electronic structure. Knowing this fact, the different metal ions doping in the carbon nitride lattice and their relative effect on structural and optical properties have been planned. We have chosen copper, cobalt and manganese as metal ions dopant and synthesized Cu, Co and Mn doped carbon nitride. The expected alteration of structural and optical properties were determined for three different metal ions doping which may be due to multiple factors including formation of defects due to doping,

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