Title : Engineering Structural Dimensionality in Copper(II) Coordination Compounds to Tune Photocatalytic Performance

Author(s) : 1. Preechayaporn Jaikead **Student ID :** 650510068

Major : Chemistry

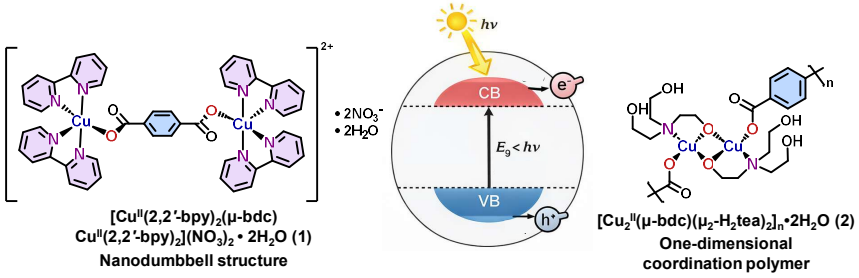
Advisor(s) : 1. Associate Professor Dr. Saranphong Yimklan
2. Assistant Professor Dr. Yothin Chimupala

Type of presentation* *(choose 1)* :

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ABSTRACT

Two novel copper coordination compounds, a binuclear complex $[Cu^{II}(2,2'\text{-bpy})_2(\mu\text{-bdc})Cu^{II}(2,2'\text{-bpy})_2](NO_3)_2 \cdot 2H_2O$ (**1**) and a one-dimensional coordination polymer $[Cu_2^{II}(\mu\text{-bdc})(\mu_2\text{-}H_2tea)_2]_n \cdot 2H_2O$ (**2**), were successfully synthesized and evaluated for photocatalytic dye degradation. The binuclear complex was prepared via a microwave-assisted method using 2,2'-bipyridine (2,2'-bpy) and 1,4-benzenedicarboxylic acid (H_2bdc), while the coordination polymer was constructed from H_2bdc and triethanolamine (H_3tea). The crystal structure indicates that **1** features a distorted octahedral geometry around the copper centers, whereas **2** consists of dinuclear Cu^{II} nodes with distorted square-planar geometry propagating into infinite one-dimensional chains through carboxylate bridges and hydrogen-bonding interactions. Spectroscopic studies confirmed metal-ligand charge transfer transitions and redox-active copper centers. Optical measurements showed band gap energies of 3.96 eV for the binuclear complex and 2.66 eV for the coordination polymer. In the photocatalytic degradation for methyl orange, **1** achieved 53% removal, while **2** reached up to 80% degradation within 90 minutes. Radical trapping indicates that hydroxyl radicals (•OH) are the key reactive species. Overall, these copper coordination materials show that their structural differences strongly influence their optical behavior and photocatalytic performance, highlighting their promising potential for practical applications in dye wastewater treatment.



$[Cu^{II}(2,2'\text{-bpy})_2(\mu\text{-bdc})Cu^{II}(2,2'\text{-bpy})_2](NO_3)_2 \cdot 2H_2O$ (1)
Nanodumbbell structure

$[Cu_2^{II}(\mu\text{-bdc})(\mu_2\text{-}H_2tea)_2]_n \cdot 2H_2O$ (2)
One-dimensional coordination polymer

Photocatalytic degradation performance comparison: 53% (1) vs 80% (2)