# Experimental and Computational Research of Graphene Quantum Dots (GQDs) for Optical Sensing of Cu Ions

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Copper ion is an essential trace element for cellular functions in both plants, animals, and human physiology. Many analytical methods have been developed to detect $Cu^{2+}$ under physiological conditions but the majority of the developed methods are costly, technically complicated and time-consuming. Graphene quantum dots (GQDs) are a class of carbon nanoparticles that are smaller than 100 nm in size. GQDs have low toxicity and tunable optoelectronic properties including photoluminescence (PL) properties, which makes them useful for sensing applications, such as copper ion detection. In this work, we investigate the origin of fluorescence quenching of Cu ion adsorption on GQDs based on a combination of state-of-the-art density functional theory (DFT) and time-dependent (TD) DFT calculations. Molecular models of GQDs are constructed on the basis of experimental XPS results, and the calculation results were analysed based on the visualization of the molecular frontier orbital (MO), electron density difference (EDD) to understand the quenching behaviour of Cu ion adsorbed GQD.