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### Rare earth doped ZnO nanoparticles: Gas sensing and photocatalytic application

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**Statement of the Problem:** Nowadays, advanced industrialization has expanded the demand for synthesis of chemical used in daily life. Growing industries promoting the environmental danger, which is an alarming threat to ecosystem. For safeguard of environment, detection of poisonus gases and release of colored waste water is required for eutrophication pollution. Researchers around the globe are trying their best efforts to save the environment. For this remediation advanced oxidation process is used for potential applications. ZnO is an important semiconductor photocatalyst with high photocatalytic and gas sensing activities. For an efficient photocatalytic and gas sensing properties, it is necessary to prepare rare earth doped ZnO compound to decrease the electron-hole recombination rates. However, rare earth doped metal oxide is seldom studied for photocatalytic and gas sensing applications. The purpose of this study is to describe best photocatalyst for photo degradation of dyes and gas sensing properties.

**Methodology and theoretical orientation:** Economical framework has to be used for synthesis of ZnO. Indepth literature survey, simple heat tretament method is utilized for gas sensing and photocatalytic activities.

**Findings:** Rare earth doped ZnO nanoparticles were best photocatalyst for photodegradation of organic dyes and different gas sensing applications by varying various factors such as pH, aging time, different concentrations of doping and co-doping metals in ZnO. Complete degradation of dye was observed only in min. Gas sensing nanodevice showed better response and quick recovery time for doped/co-doped ZnO.

**Conclusion & Significance:** In order to prevent the air and water pollution, well crystalline ZnO nanoparticles were synthesized by rapid and economic method which is used as photocatalyst for photodegradation of organic dyes and gas sensing applications to sense release of hazardous gases from the environment.

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#### Electrochemical property of carbon- based materials: first-principles and experiment

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Electric double layer capacitors, also called supercapacitors, ultracapacitors, and electrochemical capacitors, are gaining increasing popularity in high power energy storage applications. Carbon nanotubes (CNT) are carbon allotropes with cylindrical 1-D structure. CNT are consisted of either one rolled-up graphitic sheet (single- walled CNT) or several coaxial ones (multiwalled CNT). Graphene oxide (GO), an oxidized form of graphene that can be dispersed in water in single-sheet form for large-scale production, is selected as the precursor for the formation of graphene nanostructures. Reduced graphene oxide (rGO) nanosheets are extremely attractive due to their large lateral size after processing, which results in a much lower percolation threshold and fewer junctions in a continuous film, giving rise to high electrical conductivity. In this work, we make the best of the theoretical calculation demonstrated that rGO electrochemical performance is better than CNT and GO. Reported the electrochemical performance of carbon-based materials by first-principles calculation, which based on DFT were performed using CASTEP and DOML3 program (Materials Studio7.0). Additionally, we also by experiment proved rGO electrochemical performance is best. What is more, we through theoretical calculation reported that rGO is a great influence to electrochemical properties due to the abundant epoxy groups on its basal plane and the carboxyl groups at the sheet edges (Figure 1). For these purpose, rGO with unique structure and outstanding properties will become the intriguing carbon materials in supercapacitors, owing to (1) avoid  $\pi$ - $\pi$  stacking and van der Waals interactions; (2) the application of electrochemical may be controlled by adjusting content of oxygen;(3) contain tiny amounts band gap can vastly enhance the potential in various applications.

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