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## **CO<sub>2</sub> Adsorption by Nitrogen-Doped Carbons Prepared from Biomass Soybean**

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Nitrogen-doped activated carbon was synthesized by protein source from biomass soybean. Soybean is a significant and cheap source of protein which is nitrogen base compound. This work is intended to new carbonaceous adsorbents with nitrogen content in the carbon framework that applying CO<sub>2</sub> capture. The activated carbon was characterized using X-ray diffraction, scanning electron microscopy, energy dispersive X-ray spectroscopy and Fourier-transform infrared spectroscopy. Characterization results show nitrogen and oxygen functional group in activated carbon. This adsorbent has sufficient porosity whit high content of nitrogen (12 % wt.) makes it one of suggestion for CO<sub>2</sub> capture. The experimental value of adsorption modeled by Langmuir adsorption isotherm and good agreement capacity. The synthesized activated carbon demonstrates high CO<sub>2</sub> capture with 3.21 mmol/g at 25 °C and 2 mmol/g at 50 °C. The results showed that nitrogen doped of carbons can be used as potential adsorbent for CO<sub>2</sub> capture.

**Keywords:** Activated carbon, Carbon dioxide, Nitrogen, Soybean, Adsorption.

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### **Comparative Investigation of Some Selected Properties of Mn<sub>3</sub>O<sub>4</sub>/PbS and CuO/PbS Nanocomposites**

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In this paper, a comparative study of Mn<sub>3</sub>O<sub>4</sub>/PbS and CuO/PbS nano-composites deposited by chemical bath deposition method has been made using X-ray diffraction, scanning electron microscope, Rutherford back scattering, UV-visible spectroscopy and four point probe techniques. Structure of both nanocomposites were observed by XRD technique. The crystallite size for Mn<sub>3</sub>O<sub>4</sub>/PbS and CuO/PbS nanocrystalline films were found to be 34.86 nm and 19.14 nm, respectively. The surface morphology of both composites were observed by SEM technique. Mn<sub>3</sub>O<sub>4</sub>/PbS films showed non-uniform irregular spherical particles spread across the substrate surface, whereas CuO/PbS thin films showed uniform grains with dense structure which are well covered to the substrate with rod like structure. Both films have high absorbance exhibiting a maximum in the UV region. The direct band gaps of 3.90 and 3.95 eV were observed for Mn<sub>3</sub>O<sub>4</sub>/PbS and CuO/PbS films, respectively. The wide band gap values are in the range suitable for use as window materials in solar cell fabrication and high frequency applications.

**Keywords: Mn<sub>3</sub>O<sub>4</sub>/PbS, CuO/PbS, Grain size, Band gap, Nanocomposites.**

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### **First-Principles Study on Structure and Properties of $\text{Cu}_n\text{Zn}$ ( $n = 1-12$ ) Clusters**

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An all-electron scalar relativistic calculation on  $\text{Cu}_n\text{Zn}$  ( $n = 1-12$ ) clusters has been performed by using density functional theory (DFT) with the generalized gradient approximation (GGA) at PW91 level. Present results showed that the lowest energy geometry of  $\text{Cu}_n\text{Zn}$  ( $n = 1, 3, 4, 6-12$ ) clusters can be generated by substituting Zn atom for one Cu atom of  $\text{Cu}_{n+1}$  cluster and add Zn to  $\text{Cu}_n$  cluster. The ground state structures of  $\text{Cu}_2\text{Zn}$  and  $\text{Cu}_5\text{Zn}$  clusters vary significantly. Due to their electronic structure,  $\text{Cu}_2\text{Zn}$  is linear structure and  $\text{Cu}_5\text{Zn}$  is three-dimensional structure, but  $\text{Cu}_3$  and  $\text{Cu}_6$  are planar structures. Compared with the corresponding pure  $\text{Cu}_{n+1}$  cluster, the lowest energy geometry of  $\text{Cu}_n\text{Zn}$  cluster is slightly distorted. Cu-Zn bond in  $\text{Cu}_n\text{Zn}$  clusters is weaker than Cu-Cu bond in pure  $\text{Cu}_{n+1}$  clusters, and most of the Cu-Cu bonds far from Zn atoms in  $\text{Cu}_n\text{Zn}$  clusters are strong than Cu-Cu bond in pure  $\text{Cu}_{n+1}$  clusters. After doping with Zn atoms, the second-order difference of energy for  $\text{Cu}_n$  clusters produces a significant parity conversion phenomenon.

**Keywords:** Copper cluster, Scalar relativistic calculation, DFT, catalytic property.

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### **Preparation of Chlropyrofos Loaded Silver Nanoparticles Coated with Poly(ethylene glycol) and Chitosan and Evaluation of Termiticide Activity**

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A delivery system of insecticides induces active ingredient having desirable for pest control and nanotechnology may be improve of pesticide efficiency. Chlropyrofos as an organophosphate insecticide is used to control many different type of agricultural pest such as termites, mosquitoes, cockroaches. Termites, one of the important pests, cause a lot of damages to many field of agricultutre and in the south of Iran, subterranean termite, is popularly damages many products. In this research, chlropyrofos was loaded onto poly(ethylene glycol) and chitosan decorated nanoparticles (silver/PEG/Cts NPs) and evaluated its insecticidal (termiticide) study. Silver nitrate was used as the silver source and chitosan and PEG were used as the polymeric supporter and stabilizer and chlropyrofos as insecticide. The developed Ag/PEG/Cts NPs-chlropyrofos were then characterized by a UV-VIS spectrophotometer, Fourier transform infrared, transmission electron microscope, confirmed the formation of spherical nanoparticles with the size of 15-25 nm. The insecticidal activity of nanoparticle was tested *in vitro* against termite (*Microcerotermes gabrielis* W. (Isoptera: Termitidae)). The result showed the effectiveness of the target nanoparticles after 48 h at 50 ppm on the insects.

**Keywords: Amino acid, Ultrasound, Aqueous media, Cavitation.**