Title: ***Synthesis and Characterization of ZrO_2 - BiOBr Nanocomposites for Photocatalytic Degradation***

Objective:

- To study the photocatalytic degradation of Zirconia - Bismuth oxybromide (ZrO_2- BiOBr) Nanocomposites.
- Investigate the excellent properties of nanocomposites for the degradation reactions of organic pollutants.

Significance of work:

Nowadays, the development of highly visible-light active photocatalysis materials has attracted tremendous amount of interest. Zirconium oxide (ZrO_2) known as zirconia is an interesting material due to its application in various photochemical heterogeneous reactions. Zirconia is an n-type semiconductor with a wide band gap energy between 5.0 and 5.5eV. Because of this, ZrO_2 requires UV light (<280nm) to excited and generate electron-hole pairs. A strategy to overcome this is by doping ZrO_2 coupling with other metal oxides with dissimilar band edge. Composites made of two metal oxides have attracted much attention in different researches because they possess improved physicochemical properties than the pure oxides. Usually, composites enhance photocatalytic activity, produce new crystallographic phases with quite different properties than the original oxides, create defect energy levels in the band gap region, change the surface characteristics of the individual oxides due to the formation of new sites in the interface between the components, and also increase the stability of a photoactive crystalline phase. Recently, Bismuth oxyhalides (BiOX, X=Br) exhibited excellent photocatalytic activity owing to their special layered-structure composed of halogen atoms. Their excellent properties as a semiconductor material, especially for the degradation reactions of recalcitrant organic pollutants. Bismuth oxybromide (BiOBr) has attracted growing attention due to its suitable band gap (~2.7eV) and charge transfer ability. However, the practical application was inhibited due to the rapid recombination of photo induced charge carriers. In order to improve photo-catalytic activity. To enhance the photocatalytic activity of Zirconia doped with Bismuth oxybromide ($ZrO_{2\,-}$ BiOBr) nano-composites has been associated with the changes in their structural and optical properties, such as surface area, particle size, formation of a specific crystalline phase, and band gap.

Methodology:

1. **Synthesis of BiOBr:**
   Firstly, Bi $(NO_3)_3 \cdot 5H_2O$ should to dissolve into ethyl alcohol under magnetic stirring. After being stir for 10 min, tetrabutyl ammonium bromide was added drop into the above solution slowly.

2. **Synthesis of ZrO_2:**
   Zirconium (IV) butoxide added drop wise to deionized water and ethanol mixture pre-heated at 70°C. Before adding of the alkoxide, pH was to be adjust at 3 with hydrochloric acid. The white suspension kept under temperature at 70°C, with continuous stirring and reflux for 24h. The gel was let dry at 70°C for 8h. Finally, the obtained powder have calcined at 500°C for 4h.

3. **Synthesis of ZrO_2 - BiOBr:**
   At the same time, ZrO_2 powder was then to be added into the mixture above BiOBr solution under stirring until complete dissolution. The resulting solution was transferred to a Teflon-sealed autoclave and maintaining at 120°C for 6h. After cooling down to ambient temperature and centrifuging, the powder to be wash with deionized water and ethyl alcohol. Following by desiccation an oven at 60°C for 8h to get the nanocomposites powder.

Characterization:

ZrO_2-BiOBr crystalline phase, morphology, chemical composition and optical property of the photocatalyst nanocomposites will be characterizing by physico-chemical techniques such as X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscope (SEM), transmittance electron microscopy (TEM), Fourier transform infrared (FTIR) spectrometry and photoluminescence (PL) spectra. To estimate band gap energies of the photocatalyst nanocomposites use to UV-Vis spectroscopy.

Result:

ZrO_2 - BiOBr nanocomposites will be in order to enhance photocatalytic performance compared to their pristine moieties Compared with pure zirconia, the enhanced photocatalytic performance of ZrO_2- BiOBr was ascribed to the doping of BiOBr acted as trapping center. The photo degradation of organic pollutant samples in the experiments show that ZrO_2-BiOBr revealing excellent stability and recyclability. The free radical scavenging experiments revealing that $\bullet O_2^-$ and h^+ play key roles in the photocatalytic process. Therefore, the ZrO_2- BiOBr is a promising candidate for organic pollutant photo degradation caused by various industries. ZrO_2 - BiOBr nanocomposites studies will be provided promising photocatalysts results.

Reference:

1. Qiuping Yang, Yubo Zhai, Ting Xu, Kexian Zhao, HuizhiL, 'Facile fabrication of Sc-BiOBr photocatalyst immobilized on palm bark with enhanced visible light photocatalytic performance for estradiol degradation'. Journal of Physics and Chemistry of Solids: **130**, 127 - 135 (2019).

2. M. C. Uribe López, M. A. Alvarez Lemus , M. C. Hidalgo, R. López González , P. Quintana Owen, S. Oros-Ruiz, S. A. Uribe López and J. Acosta, 'Synthesis and Characterization of ZnO-ZrO_2 Nanocomposites for Photocatalytic Degradation and Mineralization of Phenol'. Journal of Nanomaterials: 12 pages (2019).