J Nanomed Nanotechnol 2016, 7:6 (Suppl)
http://dx.doi.org/10.4172/2157-7439.C1.047

Facile synthesis of SiO_2@TiO_2@Ag_2O composite catalyst for degradation of RhB dye under UV and visible light

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Herein, the thin layered n-type TiO_2 semiconductor is coated on SiO_2 spherical particles followed by decorating p-type Ag_2O nanoparticles outside with the purpose of p-n heterojunction formation for effective electron and hole separation. The composite spherical particles abbreviated as SiO_2@TiO_2@Ag_2O was characterized by XRD, SEM, TEM, HRTEM, and DRS techniques. The catalytic performance was tested for degradation of RhB dye under UV and Visible light sources. The composite catalyst showed an excellent RhB dye degradation. The combined n-type TiO_2 with the rich in electron inward and the p-type Ag_2O with the rich in hole outward facilitates the degradation reaction of dye. Therefore, n-type TiO_2 inside and p-type Ag_2O outside on the surface of SiO_2 support can be used as a catalyst for effective degradation of organic dye.

Keywords: p-n heterojunction, catalyst, degradation, nanoparticles, RhB dye.

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A coarse-grained molecular dynamics study on the mechanical properties of multi-layer graphene

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Graphene is the thinnest, hardest and toughest material known. Multi-Layer Graphene (MLG) and other graphene assemblies are important aspects of graphene application for their outstanding properties. Coarse-grained molecular dynamics (CG-MD) methods are developed to investigate the behavior of MLG and graphene assemblies due to the limitations of experimental observations and full atom simulation. In this paper, the CG-MD method based on Tersoff potential is used to simulate MLG. Besides the obvious reduction in calculation amount, only the coordinates of the model are needed in the process of computation, which greatly reduces the time of modeling and makes it easier to build complicated models. The comparison between the results of full atom model and CG-MD model is made. It is proved that the CG-MD model can predict the behavior of MLG accurately. It has great significance to produce graphene fiber with high performance.

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