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Combined Experimental and Computational Approach to Develop Efficient Photocatalysts Based on RE-TiO_2 Nanoparticles

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Extended Abstract

Taking into consideration the current socioeconomical and environmental situation, new environmentally friendly and efficient nanomaterials that can degrade organic pollutants are needed. Semiconductor-based heterogeneous photocatalysis is a versatile, low-cost, clean and environmentally benign treatment technology for a variety of pollutants. Of high interest are TiO_2-based nanomaterials, which can offer promising avenues for innovative applications such as environmentally friendly photocatalysts. It has been demonstrated to promote the decomposition of a variety of organic and inorganic compounds in both the gas and liquid phases, prompting its potential application in sterilization, sanitation and air and water purification systems. A serious drawback of TiO_2 is that it can only be excited by ultraviolet light (<5% of the solar irradiation) due to its relatively large band gap (about 3.2 eV). Therefore, development of visible light (Vis) active photocatalysts to efficiently utilize solar energy is both an important and challenging research field. Reactivity of TiO_2 in visible light (λ>400 nm) can be achieved in several ways, including metal doping or surface modification by earth rare-metal nanopraticles (RE).

This study has demonstrated for the first time the potential benefits of using computational approach supporting experimental methods to obtain predictive knowledge on structural features of Re-TiO_2 nanotubes (RE-NTs) that may govern their photocatalytic activity under visible light. In this work, the influence of the type of rare metal (Re) on the electronica properties as well as on their photocatalytic activity, were investigated by combined experimental–theoretical approach. RE-NTs was prepared via an electrochemical method. The RE-NTs photocatalysts were characterized experimentally (i.e. by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), UV–Vis absorption, scanning electron microscopy (SEM) and luminescent spectroscopy)). The obtained results indicated that toluene in the gas phase was successfully degraded under visible light (LEDs λ_{max}= 465 nm) using RE-NTs. Based on experimentally obtained results we selected most active sample (Ho-NTs). To investigate the electronic properties that can be responsible for higher photocatalytic activity of surface modified Ho-NTs computer simulations were performed. Molecular models of Ho-NTs were optimized using the plane-wave-based Vienna *ab-initio* simulation package (VASP) implementing spin-polarized density-functional theory (DFT) and the generalized gradient approximation (GGA). Based on experimental result (supported by computational methods) is proposed that during the electrochemical process, TiO_2 systems with new Ho-f states below the conduction band of TiO_2 is formed. The photocatalytic activity under Vis irradiation is attributable not to •OH but to other forms of reactive oxygen species (O_2•−, HO_2•, H_2O_2).

It should be highlighted, that the methodology presented here can serve as an important starting point for the further design of new photocatalysts with enhanced functionality supported by computational methods.

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