

Photocatalytic Activity of Er-TiO₂ Nanocomposite

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Extended Abstract

One of the directions in the evolution of the environmental friendly technologies is developing efficient methods of contaminant disposal. Particularly, researchers pay attention to the semiconductor-based heterogeneous photocatalysis that plays a crucial role in degradation of impurities in the presence of TiO₂ nanomaterials. At present, the methods based on photodegradation are widely used during purifications of water streams and wastewater, as well as to remove volatile substances from the atmosphere. This approach uses commonly available resources of solar radiation and simultaneously does not require additional chemicals during purification, what is a huge advantage over any other conventional methods.

The photocatalytic property of TiO₂ is closely related with the band gap energy. When the semiconductor (TiO₂) is exposure on the solar radiation, the photon $h\nu$ with the energy equal or greater than the band gap of TiO₂ (~3.2 eV) creates electron-hole pair – the valence electron is excited and promoted to conduction band, while the positive hole is formed on the valence band. This metastable state can be recombine and release the energy as a heat or in reaction with surrounding electron donors/acceptors (causing their degradation at the same time) or as a result of interactions with the surrounding double layer of the particle. The minimum energy to performed electron-hole pair (~3.2 eV) corresponds to the photon energy at a wavelength of $\lambda > 388$ nm, what is 3-5% of solar radiation. The main drawback of application of TiO₂ NPs as environmentally benign treatment technology for a variety of pollutants is that it can only be excited by ultraviolet light. Thus, an extension of its absorption wavelength range to the visible region (vis) is desirable to use the main part of solar spectrum. One of the most promising approach for extension of the spectral sensitivity is to influence electronic properties of TiO₂ by some structure modifications. In this way, it is possible to get an efficient photocatalyst activated of UV, Vis and NIR radiation. Reactivity of TiO₂ in visible light ($\lambda > 400$ nm) can be achieved by: (i) transition metal ions doping (e.g. Cr, Mn, Mo, Nb, V, Fe, Ru, Au), (ii) non-metals doping (e.g. N, S, B, F, I), (iii) reduced form of TiO_{2-x}, or (iv) doping with semiconductors, which have lower band gap energy. Recently, researchers provide potentials for TiO₂ photocatalysts modified lanthanides, for example holmium atom [1]. The modified titanium dioxide nanomaterial can form the basis for the new generation semiconductor. The aim of the project is to develop the TiO₂-based semiconductor having photocatalytic activity under visible ($\lambda > 380$ nm) and NIR ($\lambda > 780$ nm) radiation. This study has demonstrated application of the plane-wave-based Vienna ab-initio simulation package (VASP) to obtain predictive knowledge on structural features of RE-TiO₂ nanoparticles (RE - rare earth metal) that may govern their photocatalytic activity. The main aim of presented research was to develop molecular models of surface modified TiO₂ NPs with erbium (Er-TiO₂) useful in description of relationship between Er structure and electronic properties of surface modified TiO₂-based system. The knowledge about the influence of Er on photocatalytic activity TiO₂ can help in the design of new generation semiconductor in the future.

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References

- [1] P. Mazierski, J. Nadolna, “Enhanced photocatalytic properties of lanthanide-TiO₂ nanotubes: An experimental and theoretical study,” *Applied Catalysis B: Environmental*, vol. 205, pp. 376-385, 2017.