COMPUTATIONAL AND OPTOELECTRONIC STUDIES OF RARE EARTH METALS DOPED TITANIA FOR PHOTOCHROMIC APPLICATIONS

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ABSTRACT

Nanofabrication of TiO_2 makes it useful in varieties of applications like photocatalysis, photochromic devices, self-cleaning coatings, fog proof glass and water purifier. Titanium (IV)-oxide occurs in nature in three mineral forms: anatase, brookite and rutile. All three forms are characterized with high refractive index, low absorption and low dispersion in visible and near-infrared spectral regions, high chemical and thermal stabilities. This important metal-oxide semiconductor with relatively wide band gap (3.25 eV for anatase, 3.0 eV for rutile, 1.9 eV for brookite) and low phonon energy (<700 cm^{-1}) is an excellent host for various rare earth (RE) impurities providing their efficient emission in visible range. These systems are of possible interest in white light emission diode (LED) industry, photocatalysts and photochromic applications. At the same time, being non-toxic and biocompatible, rare-earth doped anatase has strong potential to replace standard types of fluorophores (quantum dots, organic dyes, etc.), traditionally used as fluorescent markers in medicine and biological applications. Titanium and Rare earth doped TiO_2 nanoparticles will be synthesized by sol gel and wet precipitation method. Theoretical optical properties will be estimated by density functional theory (DFT) using quantum EXPRESSO software, which will be corroborated with experimental data. Morphological and structural properties will be characterized by Scanning electron microscope (SEM), transmission electron microscope (TEM) Energy dispersive X-ray (EDX), X-ray diffraction (XRD), UV-visible spectroscopy, Fourier Transform infrared (FTIR) spectroscopy and photolumnisce spectroscopy.

ABBREVIATION AND ACRONYMS

LED	Light emission diode
RE	Rare Earth
DFT	Density Functional Theory
SEM	Scanning electron microscope
TEM	transmission electron microscope
XRD	X-ray diffraction
NPs	Nanoparticles
NCs	Nanocrystals
TMOs	Transition-metal oxides
CB	conduction band
VB	valence band