Experimental study and quantum chemical modeling on the effect of tin impurity sites in titanium dioxide on its electronic properties

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Doping titanium dioxide with different metals is effective method for change of its properties in particular photocatalytic. Mesoporous nanocomposite materials based on TiO_2 with different tin content were synthesized using titanium (IV) tetrabutoxide, $SnCl_2$, citric acid and castor oil. The energy-dispersive spectroscopy based on energy-dispersive technique proves that these materials have a uniform distribution of Ti, Sn and O. All the composite samples revealed weak peaks which belong to the anatase phase and intense peaks corresponding to the rutile phase.

The Sn/TiO_2 samples are fragmented agglomerates (Fig. 1). Examination of these powders by means of energy-dispersive spectroscopy based on energy-dispersive technique proves that materials include the elements Ti, O, and Sn (Fig. 1).

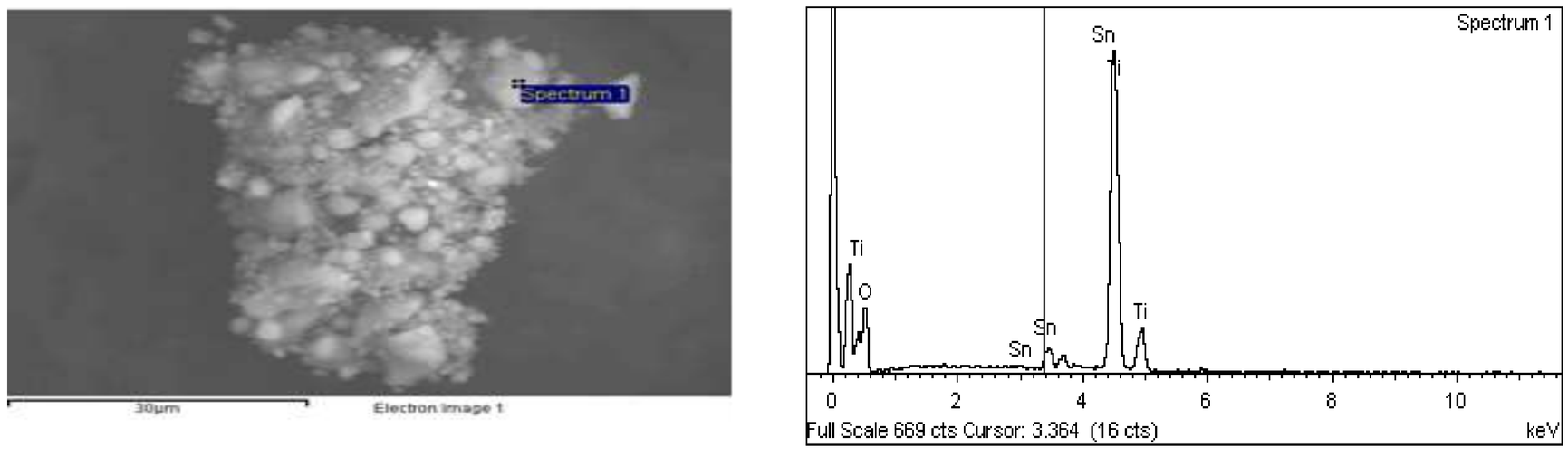

Fig 1. SEM images and energy-dispersive spectrometry (EDS) spectrum of $2Sn/TiO_2$

Equilibrium spatial structures of the anatase-like model clusters $Sn_{14}H_{22}O_{39}$, and $Ti_{14}H_{22}O_{39}$ as well as of the clusters including 1, 2, or 3 impurity tin atoms are shown in the Fig. 2.

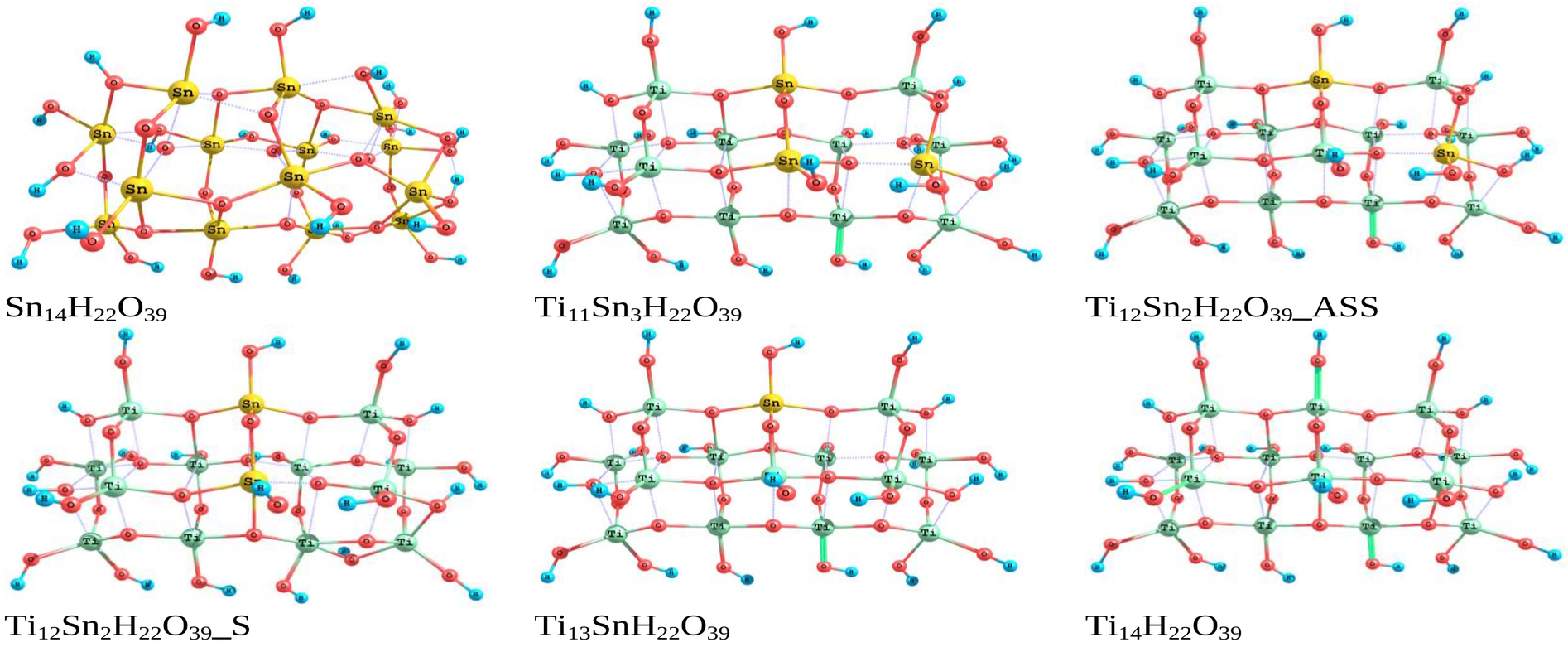

Fig. 2. Spatial geometry of the anatase model with various number of Sn atoms

Absorption spectra of nanocomposites showed a bathochromic shift as compared with the absorption band of pure TiO_2 (Fig 3) and band gap narrowing. Nanocomposites Sn/TiO_2 exhibit higher photocatalytic activity than pure TiO_2 in the reactions of dyes (Safranine T, Rodamine B) photodestruction in water solutions and photocatalytic hydrogen evolution from alcohol-aqueous solutions.

Fig. 3. UV-Vis diffuse reflectance spectra of samples: 1 – TiO_2 2 – $0.1Sn/TiO_2$, 3 – $0.5Sn/TiO_2$, 4 - $1Sn/TiO_2$, 5 - $2Sn/TiO_2$