

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 TiO₂ with different tin content were synthesized using titanium (IV) tetrabutoxide, SnCl₂, 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/TiO₂ 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).

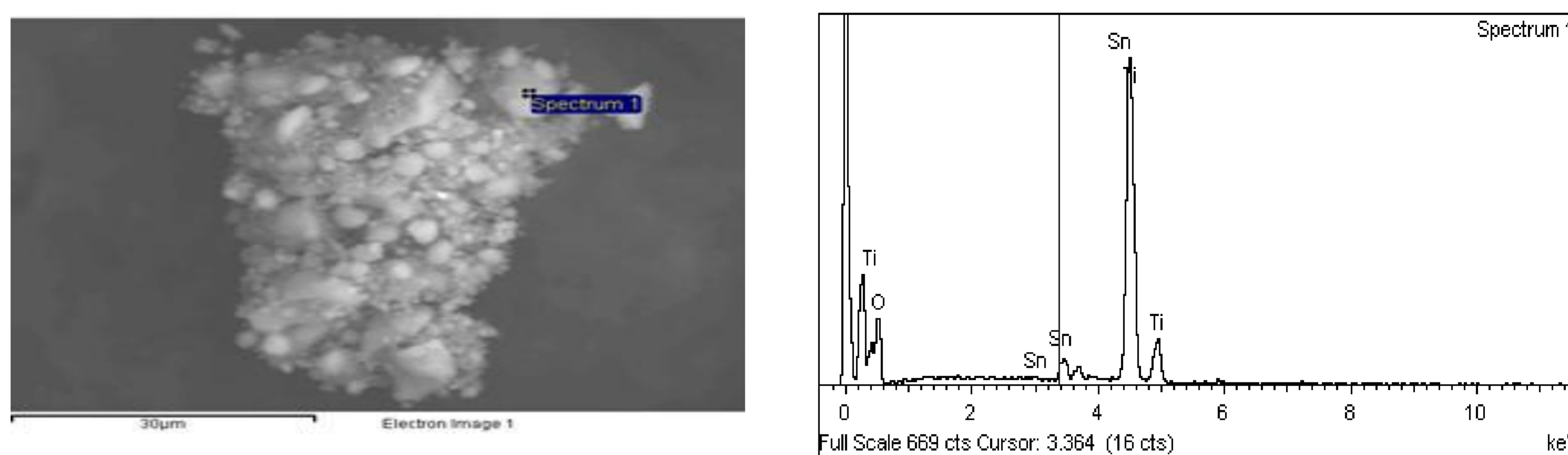


Fig 1. SEM images and energy-dispersive spectrometry (EDS) spectrum of 2Sn/TiO₂

Equilibrium spatial structures of the anatase-like model clusters Sn₁₄H₂₂O₃₉, and Ti₁₄H₂₂O₃₉ as well as of the clusters including 1, 2, or 3 impurity tin atoms are shown in the Fig. 2.

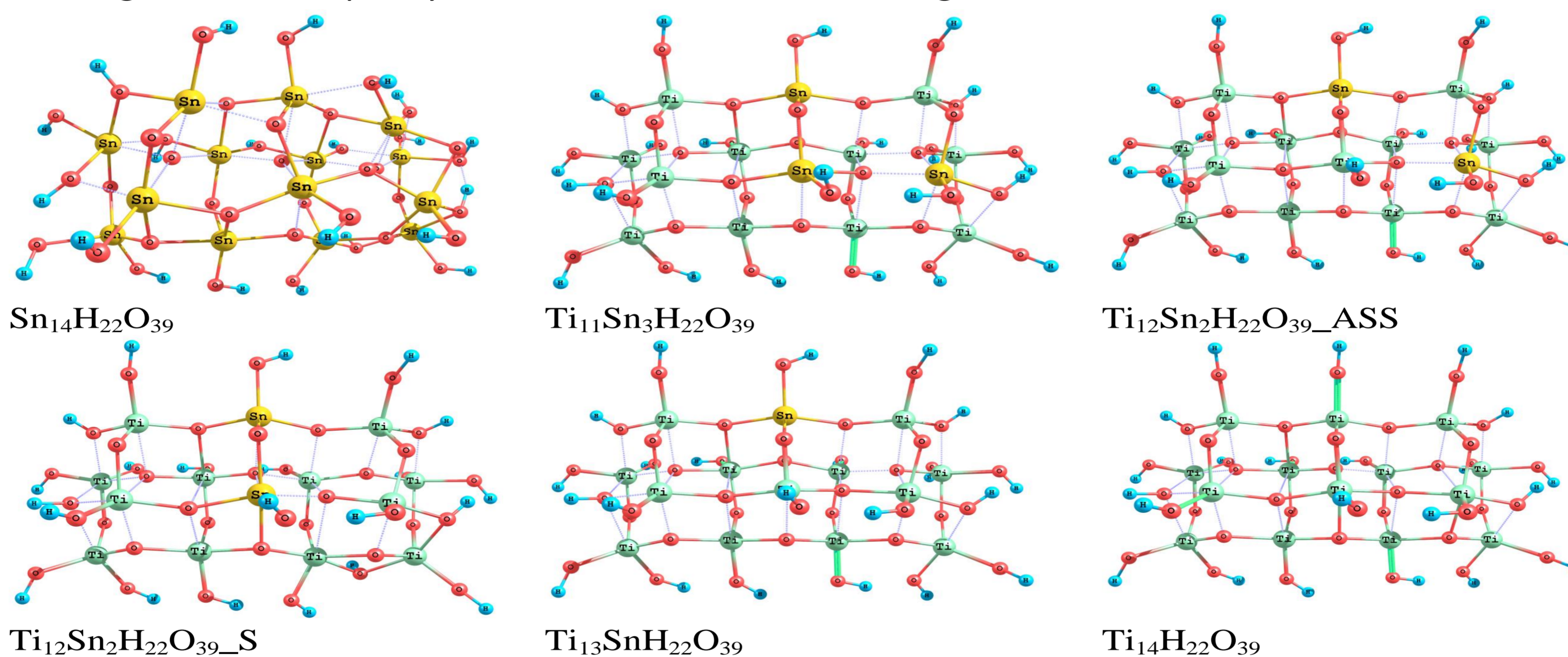


Fig. 2. Spatial geometry of the anatase model with various number of Sn atoms

Absorption spectra of nanocomposites showed a bathochromic shift as compared with the absorption band of pure TiO₂ (Fig 3) and band gap narrowing. Nanocomposites Sn/TiO₂ exhibit higher photocatalytic activity than pure TiO₂ in the reactions of dyes (Safranin T, Rodamine B) photodestruction in water solutions and photocatalytic hydrogen evolution from alcohol-aqueous solutions.

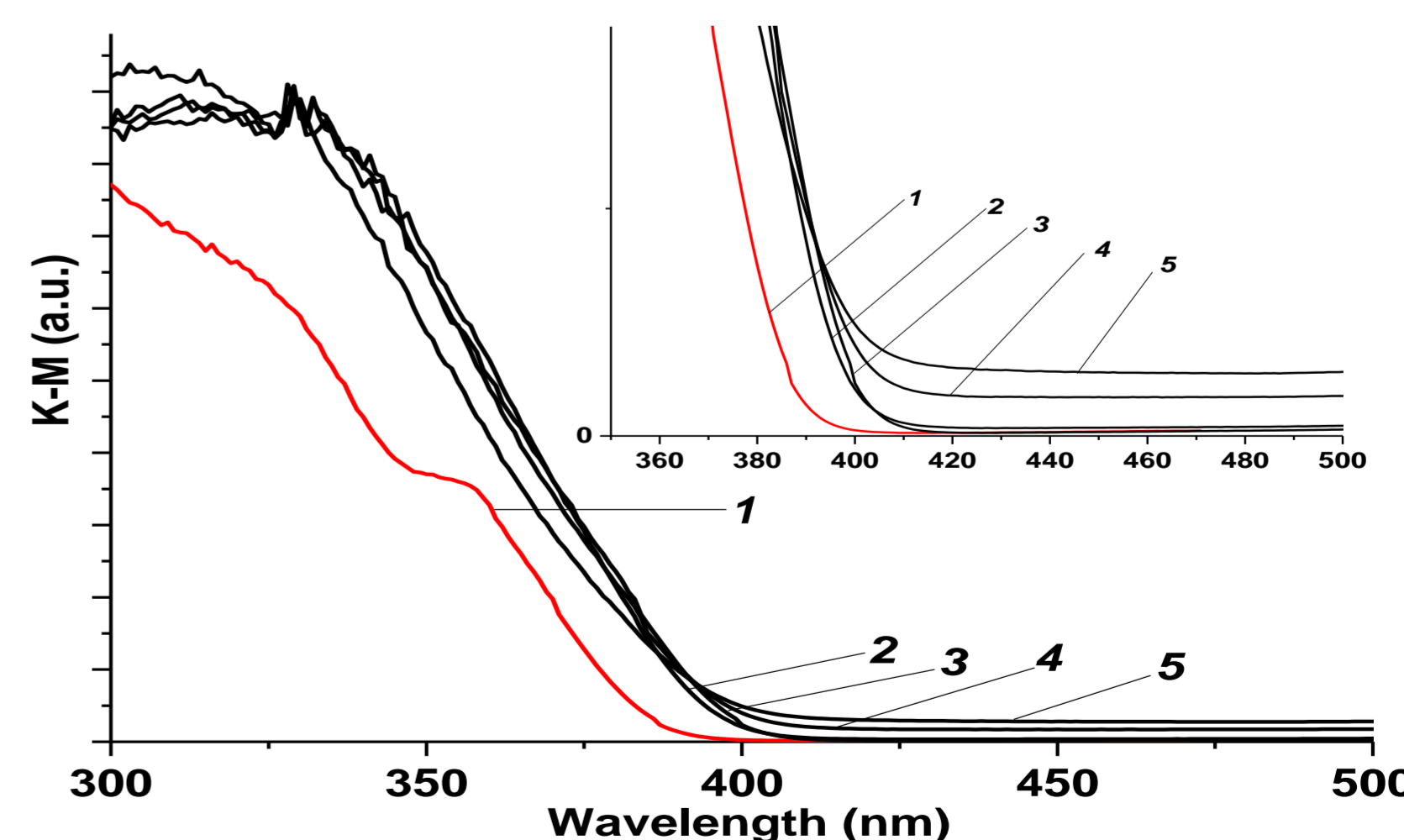


Fig. 3. UV-Vis diffuse reflectance spectra of samples: 1 – TiO₂, 2 – 0.1Sn/TiO₂, 3 – 0.5Sn/TiO₂, 4 - 1Sn/TiO₂, 5 - 2Sn/TiO₂



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