Cobalt impurity in thin dioxide and its influence in hydrogen sensors

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The structure and defects of cobalt doped tin dioxide were investigated using the density functional theory [1]–[4]. The computations were carried out for different concentrations of cobalt (3.125, 6.25, 12.5, and 18.75 at%). It is shown that at the cobalt doping less than 4 at%, the oxygen vacancy occurs at the place of the oxygen bounded by cobalt. It is energetically favorable for oxygen vacancy to occur at the nearest place to cobalt atom. The vacancy forms on the same octahedral. The electron density of states is computed when cobalt creates the states near a conduction band. By further increase in the cobalt concentration, the order of the structure begins to destroy. The structure order of tin dioxide cell is decreased in the case of 12.5 and 18.75% (in atomic percents) cobalt doping.

In the different environment conditions, surface structure changes. The number of oxygen vacancies is increased. This means that reactivity of the surface is changes, and different gases can by adsorped or detected. The adsorption of hydrogen milecule was investigeted by Density Functional Theory. It was found, that the surface is more sensitive to hydrogen molecule, in the case of 3.125 % cobalt doping, than in the undoped case. This result is in common with the experimantal researches [5].

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