ABSTRACT

The γ-Al_2O_3 and $Ce^{3+}Cu^{2+}$-doped γ-Al_2O_3 powders have been synthesized by sol-gel method. Phases of the synthesized powders were characterized with X-ray diffraction. Morphological analysis and elemental composition of the samples were determined by scanning electron microscopy, high-resolution transmission electron microscopy and energy dispersive X-ray spectroscopy. Luminescence characterizations have been used to study the synthesized samples. Ab initio calculations by the use of local density approximation with the Hubbard U correlation were used to compute the structural, electronic and optical properties of γ-Al_2O_3 and Al_2O_3:$Ce^{3+}Cu^{2+}$. The results indicate that the particle size and morphology of the samples depend on the concentration of the dopants. In comparison with undoped γ-Al_2O_3 sample, the intensities of emission peaks at 430 and 458 nm of $Ce^{3+}Cu^{2+}$-doped γ-Al_2O_3 powders have been enhanced. This shows that, increasing Ce^{3+} and Cu^{2+} concentration causes an increase in the number of emitting ions which is expected in order to increase the number of applications of γ-Al_2O_3:$Ce^{3+}Cu^{2+}$ composite powders. The photoluminescence spectrum detected at λex = 253 nm shows a new peak located at 549 nm due to Cu^{2+} ions. This was confirmed computationally when the Ce_4f and Ce_5d states are found in the conduction band while the Cu_4p state was found at conduction band minimum and Cu_3d state at valence band maximum. This location of states showed there is no possible luminescence from the Ce^{3+} ions. The only possible luminescence was due to transition from Cu_4p to Cu_3d states.