Computational study of Fe-doped TiO2 nanoparticles

B. BEZZINA, C.E. RAMOUL, K.E. SLIMANI, O. GHELLOUDJ, M.T. ABED GHARS, M. Kahalerras, H.Bendjama, D.E. KHATMI

Abstract: The geometries, relative stabilities, and electronic properties of small TinO2n (n= 1–4) clusters that are utilized in renewable energy, solar energy (as an active semiconductor metal oxide) were investigated by using density functional theory (DFT) at the B3LYP/LanL2DZ level of theory, as well as the effects of doping of different iron concentrations on the properties of titanium dioxide were given, which some Ti atoms were replaced with Fe atoms. The effects of the size and the concentration of iron all were shown to have a significant influence on the behavior of adsorption of TiO2 in the field of UV-vis. It was found out that the increase in the size of nanoparticle was accompanied with a reduction in energy of formation and a stability of the clusters. Our results are in good agreement with the experimental and theoretical results available.

Keywords: Solar energy, iron doping, titanium dioxide, clusters.