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Computational Studies of Ru and Sr-doped anatase TiO₂ on three low index surfaces for application on DSSCs

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Abstract content
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Titanium dioxide (TiO₂) is considered very close to an ideal semiconductor for photocatalysis because of its high stability, low cost and safety toward both humans and the environment. Therefore doping TiO₂ with different element has attracted researchers as the most important way of improving the width of the band structure and the adsorption on different wavelength region in order to improve the efficiency of catalytic activity and conversion. In this work we are focusing on how to enhance the efficiency of DSSCs using the density function theory (DFT) technique. We firstly vary the distance between the anatase TiO₂ surface and the added atom Ru. Each Ru-doped anatase TiO₂ (100) and (110) surfaces were optimized in order to get the total energies and structure to see the effect of the separation between the defect and the surface of TiO₂. Secondly we take the system that gives the least energy and calculate their properties, i.e. density of state (DOS), Band gaps and optical. Our results shows that the band gaps of pure anatase TiO₂ (100) and (110) surfaces are greater than the band gaps of Ru-doped anatase TiO₂ (100) and (110) surfaces. Which means that the Ru-doped anatase TiO₂ (100) and (110) surfaces have the high photocatalytic activity than pure TiO₂, because the larger the band gap, the greater the difficulty for the valence electrons to jump to the conduction band, thus explains poor electricity conductivity of non-metals.

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