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COMPUTATIONAL SIMULATION MODEL FOR DYE ADSORPTION IN NANO TIO2 FILM FOR THE APPLICATIONS IN DYE SENSITIZED SOLAR CELLS

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Abstract

The theoretical and computational studies of dye sensitized solar cells (DSSCs) can contribute to a deeper understanding of these types of solar cells. The DSSCs are the novel design of solar cells which could be used as power producing windows or skylights. They represent a particular promising approach to a direct conversion of sunlight into electrical energy at low cost and with high efficiency. The light adsorption occurs in dye molecules adsorbed on a highly porous structure of TiO_2 film. Despite the progress in the efficiency and stability of these solar cells, there is still a room of research on some of their operational aspects that are still not understood. One process, for which there is limited information, is the time taken to upload the dye on the TiO_2 nanoporous film. The processes followed experimentally for dye uptake is by dipping the TiO_2 semiconductor electrode into the dye solution for periods of several hours to several days. However, such long dipping times are not economical for industrial production of DSSCs. The factors controlling this process are not yet fully investigated. We propose a simple model based on the Langmuir isotherms to study and understand the diffusion and adsorption of the dye molecules in TiO_2 films. Our computational modelling results show that the adsorption of dye into the TiO_2 nanotubes film is controlled by the diffusion coefficient, the adsorption-desorption ratio and the initial dye concentration. Our results show that the initial dye concentration plays an important role on the surface coverage. It is also noted that for a higher concentration shorter immersion time is needed for the sufficient surface coverage. Furthermore it is observed that for the large values of the adsorption-desorption ratio there is a delay in the diffusion of dye molecules on the surface.

Key words: Solar Cells, Dye Sensitized, Dye, Surface Coverage, Langmuir

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