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Computational study of dye adsorption in nano TIO₂ film for the applications in dye sensitized solar cells using different computational techniques

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Abstract content
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The theoretical and computational studies of dye sensitized solar cells (DSSCs) can contribute to a deeper understanding of these types of solar cells. In the current study the density functional theory and the finite element methods are used to understand the factor affecting the dye adsorption and electronic properties of the TIO₂ semiconductor as the main element of DSSCs. The light adsorption occurs in dye molecules adsorbed on a highly porous structure of TIO₂ film. The processes followed experimentally for dye uptake is by dipping the TIO₂ semiconductor electrode into the dye solution for periods of several hours to several days. To understand the process of dye adsorption on the surface of TIO₂, the DFT calculations was carried out to study the electronic structure of the ruthenium doped brookite TIO₂ surface. The factors controlling the dye uptake process are also investigated, using a simple model based on the Langmuir isotherms. Our computational modelling results show that the adsorption of dye into the TIO₂ nanotubes film is controlled by the diffusion coefficient, the adsorption-desorption ratio and the initial dye concentration.
Keywords: Solar Cells, Dye Sensitized, Dye, Surface Coverage, Langmuir

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