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DFT study of Modifications of Pt-doped TiO2 using N, for application in DSSCs

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Doping has found to be one of the most promising method to in increasing photocatalytic activity of various materials. The location and nature of the doping elements strongly affect the structural, electronic and optical properties of TiO2. To tailor the band structure and modify the photocatalytic activity of TiO2 brookite (210) surface, a pair of dopants is selected. Platinum and Nitrogen atoms are inserted in the TiO2 network as substitutional and N was also doped through absorption on the surface. The main objective behind the different locations and methods of the dopant elements are to banish the isolated unoccupied states from the forbidden region that normally annihilates the photogenerated carriers. Pt replaced Ti, N replaced O and N was also absorbed and bond with 2 coordinated O in the TiO2 brookite (210) surface network. N absorbed Pt\N TiO2 provided a suitable configuration of dopant atoms in terms of geometry and band structure. Moreover, the optical properties showed a notable shift to the visible regime. Individual dopants either introduced isolated unoccupied states in the band gap or disturbed the Fermi level and structural properties. Furthermore, the other co-doped configurations showed no remarkable band shift, as well as exhibiting a suitable band structure. Resultantly, comparing the band structure and optical properties, it is argued that Pt (at Ti) and N absorbed (at O) doped would strongly improve the photocatalytic activity of TiO2 brookite (210) surface.

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