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Density function theory study of TiO₂ Brookite (100), (101) and (210) surfaces doped with ruthenium (Ru) and Calcium (Ca) for application in dye sensitized solar cell

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Abstract content
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Since the discovery of water photolysis on a TiO₂ electrode by Fujishima and Honda in 1972, TiO₂ has attracted extensive attention as an ideal photocatalytic material because of its excellent properties such as high activity, good stability, nontoxicity and low cost. Thus, it has been widely used in the fields of renewable energy and ecological environmental protection. However, as a wide band gap oxide semiconductor (Eg = 3.14 eV), brookite TiO₂ can only show photocatalytic activity under UV light irradiation (lambda; < 387.5 nm) that accounts for only a small portion of solar energy (approximately 5%), in contrast to visible light for a major part of solar energy (approximately 45%). Therefore, how to effectively utilize sunlight is the most challenging subject for the extensive application of TiO₂ as a photocatalyst. Because of the unique d electronic configuration and spectral characteristics of transition metals, transition metal doping is one of the most effective approaches to extend the absorption edge of TiO₂ to visible light region, which either inserts a new band into the original band gap or modifies the conduction band (CB) or valence band (VB), improving the photocatalytic activity of TiO₂ to some degree. In this work, the structural optimizations, band structure, and electronic density of states of doped and un-doped TiO₂ (100), (101) and (210) surfaces were performed by using the first principles calculations based on DFT using a plane-wave pseudopotential method. The generalized gradient approximation (GGA) was used in the scheme of Perdew-Burke-Ernzerhof (PBE) to describe the exchange-correlation functional. All calculations were carried out with CASTEP (Cambridge Sequential Total Energy Package) code in Materials Studio of Accelrys Inc.

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