

**Hybrid DFT study of MWCNT/Zr-doped SrTiO<sub>3</sub> heterostructure: Hydrogen production, electronic properties and charge Carrier mediator role of Zr<sup>4+</sup> ion**

Opoku F  
Govender, Krishna  
van Sittert CGCE  
Govender PP

**ABSTRACT:**

Over the past decade, remarkable efforts have been made to design low-cost, non-toxic, stable and efficient photocatalyst for water splitting. In the present work, an effective alternative approach to enhance hydrogen production of SrTiO<sub>3</sub> was by coupling with MWCNT to form heterojunction followed by doping with Zr<sup>4+</sup> ion. The observed type-II band alignment and the polarised electric field could promote the separation of photoexcited charge carriers and photocatalytic activity of these hybrid heterostructures. The theoretical calculation revealed that Zr<sup>4+</sup> ion could act as a charge carrier mediator to transfer electrons to the SrTiO<sub>3</sub> surface. The MWCNT (6,12,18)/Zr-doped SrTiO<sub>3</sub>(100) heterostructure exhibited excellent activity due to the combined effect of MWCNT (6,12,18) and Zr-doped SrTiO<sub>3</sub>(100) monolayers compared with pure SrTiO<sub>3</sub>. This study offers a novel understanding of designing highly active and stable SrTiO<sub>3</sub>-based photocatalyst as efficient hydrogen generation material.