First-Principles Investigation of Ru- and Pt-Doped TiO₂ Brookite Surfaces

Ratshilumela Steve Dima^{1,2}, Nditsheni Eric Maluta^{2,*} and Rapela Regina Maphanga^{1,3}

¹ Council for Scientific and Industrial Research, Next Generation Enterprises and Institution Cluster, P.O Box 395, Pretoria, 0001, South Africa.

² University of Venda, Department of Physics, P/Bag X 5050, Thohoyandou, 0950, South Africa

³ University of Limpopo, Department of Physics, Private Bag X 1106, Sovenga, 0727, South Africa.

*E-mail: eric.maluta@univen.ac.za

doi: 10.20964/2020.02.61

Received: 31 May 2019 / Accepted: 31 October 2019 / Published: 31 December 2019

The electronic structures and optical properties of brookite TiO₂ (100) and (110) surfaces doped with transition metals (Ru and Pt) have been investigated by first-principles calculations based on the density functional theory, employing generalized gradient approximation (GGA). The modelled surface structures were constructed from an optimized brookite bulk structure. TiO₂ surfaces were doped with transition metals, with one Ti atom replaced by a transition metal atom. The results indicate that doping with both transition metals can narrow the band gap of TiO₂, leading to the improvement in the photo reactivity of TiO₂. The metal dopants shift the absorption to high wavelengths and improves optical absorbance in the visible and near-IR region. The surface (100) showed higher activity than (110) in both regions.

Keywords: Density functional theory; TiO₂; brookite; dye sensitized solar cell; doping

[FULL TEXT](#)

© 2020 The Authors. Published by ESG (www.electrochemsci.org). This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/4.0/>).