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The African Review of Physics is a free, open access, on-line, peer reviewed, international journal that publishes reviews, research articles, and brief communications in all branches of experimental and theoretical physics with an emphasis on originality and relevance to the basic understanding of contemporary physics and related interdisciplinary fields. In addition, the African Review of Physics publishes timely Special Issues dedicated to a rapidly developing field of physics and proceedings of conferences held in Africa.

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The African Review of Physics





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**Brief History** 

Originally named The African Physical Review, it was created in 2007 by the Abdus Salam International Centre for Theoretical Physics to improve the communication capabilities of scientists in developing nations. The journal became the official organ of the African Physical Society in January 2010.

## Scope and Coverage

The African Review of Physics is a free, open access, on-line, peer reviewed, international journal that publishes reviews, research articles, brief communications, and the proceedings of conferences held in Africa. It publishes in all branches of experimental and theoretical physics with an emphasis on originality and relevance to the basic understanding of contemporary physics and related interdisciplinary fields. In addition, the African Review of Physics publishes timely Special Issues dedicated to a rapidly developing field of physics and proceedings of conferences held in Africa.

# Kind of Information

The African Review of Physics is widely listed by libraries and other e-Journal listing organizations around the world. The African Review of Physics has now a truly international character with an increased usage worldwide. Its major readership continues to be in the highly industrialized nations of North America, Europe as well as many emerging nations. The African Review of Physics holds information on recent developments on Physics especially in Africa. It strictly deals with Metric and Field Equations, Solutions of Field Equations, important models related to Physics, Physical properties, Metric and Energy Momentum Tensor, Materials and Methods of Physics, different radiation equations, analysis of data, Law of Variation etc.

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# Electronic Properties of Catechol Adsorbed on Rutile ${\rm TiO_2}$ and ${\rm SnO_2}$ (110) Surfaces: A Density Functional Theory Study

Victor Meng'wa<sup>1,\*</sup>, George Amolo<sup>1</sup>, Nicholas Makau<sup>1</sup>, Samuel Lutta<sup>2</sup>, Maurice Okoth<sup>2</sup>
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The incorporation of organic molecules such as catechol onto TiO<sub>2</sub> substrate to enhance TiO<sub>2</sub> photocatalytic activity has led to improved Dye Sensitized Solar Cells (DSSCs) efficiency. Nonetheless, it still remains low for most practical applications hence more detailed description of the electronic structure of catechol-TiO<sub>2</sub> rutile surface, could provide insight for further improvement. In this work, adsorption of catechol on rutile TiO<sub>2</sub> and SnO<sub>2</sub> (110) surfaces has been studied using first principle methods. The study investigated the role played by catechol in varying the electronic structure of TiO<sub>2</sub> and SnO<sub>2</sub> (110) surfaces. Results obtained showed that both the clean and catechol-terminated stoichiometric (110) TiO<sub>2</sub> four layer surface had a band gap of 2.1 eV. The energy gap increased by 0.32 eV which represents an 18 % increment from 1.7 eV for clean stoichiometric TiO<sub>2</sub> to 2.02 eV dlowing adsorption of catechol molecule on the TiO<sub>2</sub> (110) rutile 5-layer surface. The highest occupied molecular orbital (HOMO) in the four and five layered catechol terminated TiO<sub>2</sub> (110) surfaces was found to be about 1 eV, above the valence band maximum coles but in SnO<sub>2</sub> it nearly overlamped with bottom of conduction band. The lowest moccunied molecular orbital

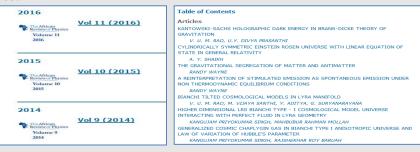
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