**Effects of π-Bridge Architecture in Organic D-π-A and Adsorption of Thiophene-Oxadiazole Dyes on TiO2 Nanocrystalline Surface for Organic Electronic Devices**

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**ABSTRACT:**

In this work, the effects of extending π-bridge and adsorption of dyes on TiO2 nanocrystalline surface on optoelectronic parameters in dyes-photosensitized solar cells (DSSCs) has ben explored. The dyes geometries, charge transference and electronic characteristics were investigated using density functional theory (DFT) and its time-dependent (TD-DFT). The impact of extended π-bridge in conjugated systems was explored, through new challenges in specific properties of Thiophene-Oxadiazole-Photosensitizers adsorbed on TiO2 nanocrystalline surface (Dyes@TiO2) under the architecture D-π-A for the organic electronic devices such as solar cells. The use of electronic excitations and reorganization energies () are viable methods for better harvesting of the solar energy and increasing its efficiency. The calculated results suggests that the HOMO-LUMO energy gap (), ionization potential (), electron affinity (), hole extraction potential (), electron extraction potential (), reorganization energies (electron and hole) (), fill factor (), open-circuit voltage (), light-harvesting efficiency (), driving force for electron injection (), driving force for dye regeneration (), density of states () are affected by Donor groups introducing in different Thiophene-Oxadiazole derivatives. Furthermore, our findings indicate that these novel designed organic photosensitizers dyes may have improved photovoltaic characteristics and are suitable applicants for efficient charge transportation in organic electronic devices.

**Keywords**: Thiophene-Oxadiazole, DSSCs, Charge Transfer, DFT/TD-DFT.

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**Biography of presenting author Dr. Simplice KOUDJINA**

Dr. Simplice Koudjina has working as an Assistant Professor in Computational Chemistry and Molecular Modeling for Nanotechnology Applications at National University of Sciences, Technology, Engineering and Mathematics (UNSTIM) in BENIN, where he works since 2018. In 2016, he holds a Ph.D degree in Theoretical Chemistry and Molecular Surface Modeling at the University of Abomey-Calavi, and M.Sc in Nanotechnology at University of Namur in Belgium in 2014. He then joined the research group of Professor Guy Atohoun in the Unit of Theoretical Chemistry and Molecular Modeling (UCT2M) at University of Abomey-Calavi (UAC) in BENIN. In 2022, he has obtained a PostDoc research stay in the group of Professor Prabhakar Chetti in Department of Chemistry at National Institute of Technology (NIT) Kurukshtra–INDIA. In 2023, he took part in several international conferences in France, USA, India, South Africa and Morocco, in the fields of Chemical Engineering and Organic Electronics Photovoltaic Devices. His field of expertise is Computational Theoretical Chemistry and Molecular Surface Modeling for Nanotechnology Applications. He has published more than 25 high research articles in impact factor journals.

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