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**DFT and TDDFT study of new molecules used in organic solar cells**

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In this work, we report a theoretical analysis on the geometries and optoelectronic properties of five new molecules used in photovoltaic cells, these compounds were studied by using density functional theory (DFT) and time-dependent (TD) calculations. The study of the structural and optoelectronic properties (HOMO, LUMO, Gap energy, Voc) is realized by using DFT method at Becke's three parameters and Lee–Yang–Parr functional (B3LYP) level with 6-31G basis set. The calculations were performed by Gaussian 09 program supported by Gauss View 5.0.8. The electronic and photo physical properties of these molecules are discussed to investigate the relationship between structure and optoelectronic properties. These properties suggest these materials as good candidates as active layer for organic solar cells.

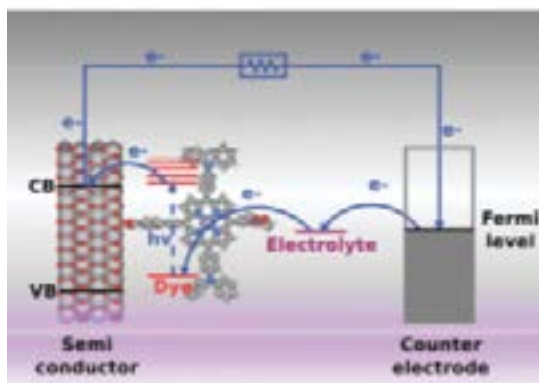


Figure 1: Schematic overview of the working mechanisms of a dye sensitized solar cell.

**Recent Publications**

1. Harper C (2009) The neuropathology of alcohol-related brain damage. Alcohol Alcohol 44(2):136-140.
2. Li X, Schwacha M G, Chaudry I H and Choudhry M A (2008) Acute alcohol intoxication potentiates neutrophil-mediated intestinal tissue damage after burn injury. Shock 29(3):377-383.
3. Sullivan E V and Zahr N M (2008) Neuroinflammation as a neurotoxic mechanism in alcoholism: Commentary on "Increased MCP- 1 and microglia in various regions of human alcoholic brain". Experimental neurology 213(1):10-17.

**Biography**

Atmani Hajar is pursuing her PhD student at the Sustainable Development Laboratory-University Sultan Moulay Slimane, Beni Mellal, Morocco. In addition she completed her master's degree in engineering of inorganic materials. Her research focuses on experimental and theoretical study of photovoltaic molecules using Gaussian software under the supervision of Dr. Ahmed Jouiat. Her thesis is based on the exploration of new theoretical inorganic molecules used in photovoltaic cells to produce electrical energy by the TDDFT method. She decided to pursue her doctorate, hoping to bring more to humanity. She also looks forward to being part of a stimulating exchange and creation of ideas in the scientific world.