# Effects of Physical Orientation of Dye Molecules and Molecular Orbitals on Performance of Solid-State Dye Sensitized Solar Cells

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## Abstract

Studies on Dye-Sensitized devices (DSDs) were initiated around late 1960s. DSDs are studied as a low cost alternative for photovoltaic optoelectronic devices, notably as solar cells. Their performance depends on the photon absorption and carrier injection properties of the sensitizer (dye). In general, the charge transfer in the molecule is based on the Donor-*π-bridge*-Acceptor (D-π-A) mechanism. Additionally, the orientation of the dye molecule affects the photon-absorption-cross-section, the injection efficiency of the carriers from the sensitizer to the semiconductor-electrode. Three variants of cyanine dyes were identified to have different orientations with respect to the $TiO_2$ surface. The current-voltage variations of the three dyes as sensitizers were studied experimentally on an *n*-$TiO_2$/Dye/*p*-CuSCN configuration. The $TiO_2$ films were prepared on fluorine-doped tin oxide (FTO) glass plates (1×1.5 $cm^2$) by hydrolyzing titanium isopropoxide slurry mixed with Degussa P25 $TiO_2$ powder. The $TiO_2$ film thickness was ~10 µm. The I-V characteristics of the cells were recorded using a calibrated halogen lamp and a KEITHELY 2400 source meter; the photocurrent action spectra was measured using a SP-DK480 monochromator and a SR-850 lock-in-amplifier set-up calibrated with a standard silicon photodiode. The absorption spectra were obtained using Ocean Optics USB2000 UV-VIS spectrometer. Additionally, a theoretical study was conducted, using the inbuilt functions in ChemDraw®, to calculate the MM2 energy minimization, identify the molecule's orientation and the HOMO and LUMO positions. The results have shown a correlation between the orientation of the dye molecule and the photocurrent of the device. Furthermore, the orientation of the dye molecule appears to be influencing the photon-harvesting efficiency and the penetration of the hole-conductor into the device. Additionally, the photocurrent results imply the MO's positions affecting the carrier transport properties of the device.