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Coumarin Dyes with Triple Bonds as π -Spacer Units for Dye Sensitized Solar Cells

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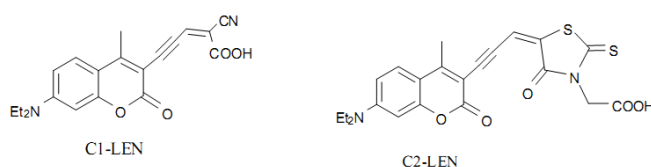
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Among metal free organic dyes studied in dye-solar cells (DSC), coumarin derivatives are a promising sensitizer for TiO₂ because of their good photoresponse in the visible region and good thermal stability under one sun soaking [1].

On the basis of concept of Donor- π -conjugation bridge-acceptor structure a series of coumarin dyes have been synthesized by inserting various numbers of thiophene or methine moieties as π bridge between coumarin as electron donor and cyano carboxylic acid as electron acceptor [2]. So far, influence of triple bond as π spacer unit in coumarin dyes has not been studied.

Here we report our recent progress in the design and synthesis of coumarin dyes (C1-LEN and C2-LEN) with triple bond as linkers between the donor and acceptor units. The chemical structures of these dyes are shown in Figure 1. Their absorption spectra and photovoltaic properties were investigated and, the electron distribution with different acceptors was performed using density functional theory (DFT) methods and time dependent DFT calculations. A complete optoelectronic characterization of obtained DSCs cells will be presented and discussed.



[1] Wang, Z.; Cui, Y.; Hara, K.; Dan-oh, Y.; Kasada, C.; Shinpo, A. "A High-Light-Harvesting-Efficiency Coumarin Dye for Stable Dye Sensitizer Solar Cells", *Adv. Mater.*, 19, 1138-1141 (2007)

[2] Hara, K.; Miyamoto, K.; Abe, Y.; Yanagida, M. "Electron Transport in Coumarin Dye Sensitized Nanocrystalline TiO₂ Electrodes", *J. Phys. Chem. B*, 109, 23776-23778 (2005).