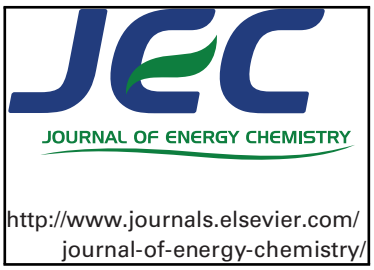

Organic dyes based on triphenylamine for dye-sensitized solar cells: Structure-property relationships#

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Organic dyes based on triphenylamine for dye-sensitized solar cells: Structure-property relationships

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Abstract

Three new organic dyes based on triphenylamine with a structure of A-D-A-D-A (**D1**), A-D-A (**D2**) and D-A (**D3**) were designed, theoretically calculated and synthesized for dye-sensitized solar cells. Dye **D1** exhibits a broader absorption than **D2** and **D3**, due to the intramolecular charge transfer between the donor triphenylamine and the acceptor benzothiadiazole. Dye **D1** exhibits a lower HOMO and a lower LUMO than **D2** and **D3** due to the electron-withdrawing benzothiadiazole. The number of anchoring group cyanoacrylic acid has no obvious influence on absorption and energy levels of **D2** and **D3**. The LUMO of **D1** locates on benzothiadiazole rather than cyanoacrylic acid anchoring groups, while the LUMOs of **D2** and **D3** are localized on cyanoacrylic acid. **D2** and **D3** give higher short-circuit current density than **D1**. **D3** with one anchoring group gives the highest open-circuit voltage. Consequently, the **D3**-based device gives the highest efficiency.

Keywords: Dye-sensitized solar cell; Organic dye; Metal-free; Triphenylamine

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