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Benzo[1,2,5]thiadiazole dyes: Spectral and electrochemical properties and their relation to the photovoltaic characteristics of the dye-sensitized solar cells

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1 **Benzo[1,2,5]thiadiazole dyes: spectral and electrochemical properties and their relation to the**
2 **photovoltaic characteristics of the dye-sensitized solar cells**

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14 **Abstract**

15 Important aspects of dye-sensitized solar cells (DSSCs) fabrication based on dyes including
16 benzothiadiazole unit were investigated. Two absorption peaks of the dyes covering the 330-551 nm region
17 and possessing moderate band energy gap (1.83 - 2.16 eV) were found to be important to demonstrate high
18 photovoltaic efficiency ($\eta > 8$) in metal free iodide/iodine electrolyte composed DSSCs. Furthermore, the dye
19 energy band gap determined from optical spectra decreases with the increase of DSSCs short circuit
20 photocurrent density, which in turn linearly increases the photovoltaic efficiency of DSSCs. While the
21 RedOx potentials of dyes are less functionally related to the photovoltaic properties of the DSSCs, their
22 appropriate values ($0.67 \leq E_{ox} \leq 1.1$ V and $-1.75 \leq E_{red} \leq -0.91$ V) can be important for efficient DSSCs.
23 Fabrication details increasing photovoltaic efficiency of the devices based on dyes with benzothiadiazole
24 unit were found. The relationships obtained in the work can be used for preliminary prognosis whether a
25 newly synthesized dye is a promising metal-free sensitizer for DSSCs or not.

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