

3-Amino-3-(pyperidine-1-yl)arylaazoacrylonitriles as sensibilizing agents for Gratzel cells

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Abstract

Rational design of dyes for pivotal Gratzel cells is solidly based on knowledge of structural electronic factors defining experimentally observed spectra. The current work applies time-dependent density functional theory approach to evaluate the potential usefulness of 3-amino-3-(pyperidine-1-yl)arylaazoacrylonitriles as sensibilizers for dye-sensitized solar cells. The energy of electron transitions observed in UV-Vis spectra for arylazoamidines strongly depends on electronic structure of substituent in aromatic ring and, thus, describes compounds which can be possibly used as sensibilizing reagents for Gratzel's solar cells.