Relationship between photo-physical and electrochemical properties of D-π-A compounds regarding solar cell applications. 1. Substituent type effect in photovoltaic performance

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Résumé en anglais	Studying the electrochemical characteristics is an important step for determining interactions between molecules and the chemical environment. Moreover, the electrochemical evaluation of dyes is highly needed to establish the behavior of electro-active chemical species inside dye-sensitized solar cells (DSSCs). Four compounds, M8-1, M8-2, M8-O1, and M8-O2 (with a common organic structure (E)-2-cyano-3-(5-((E)-2-(9,9-diethyl-7-(phenylamino)-9H-fluoren-2-yl)vinyl)thiophen-2-yl)acrylic acid), are studied in two solvents, tetrahydrofuran (THF) and dimethylsulfoxide (DMSO). Among the studied compounds, M8-1 has highlighted characteristics compared with the others: its ground and excited states oxidation potential are the highest (1.14 and −1.22 V, respectively). Also, it shows the lowest energy gap between the excited state oxidation potential and the TiO2 conduction band. Relating to the substituent effect, the shorter the length, the higher the energetic difference in the electronic transition (M8-1 and 2). Comparing characteristics through quantum chemistry, the values obtained in DMSO are the most predictable. The injection energies signal that M8-1 is the best injector. The performances in solar cells are measured in three TiO2 materials: Degussa (D-TiO2), active opaque (A-TiO2), and transparent (T-TiO2). The IPCE results show the A > T > D average tendency, and the family of substituted alkyl has higher values than the alcoxyl one. Furthermore, in the first family the methyl substituent has a higher value than the ethyl one. M8-1 has the highest IPCE value, on average. In terms of efficiency, the alkyl substituted family again has higher values than the alcoxyl family. On average, the methyl substituent has a higher value than the ethyl one in both families. M8-1 has the highest efficiency value.
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