Supplementary Material

Theoretical study of the effect of different π bridges including an azomethine group in triphenylamine based dye for dye-sensitized solar cells

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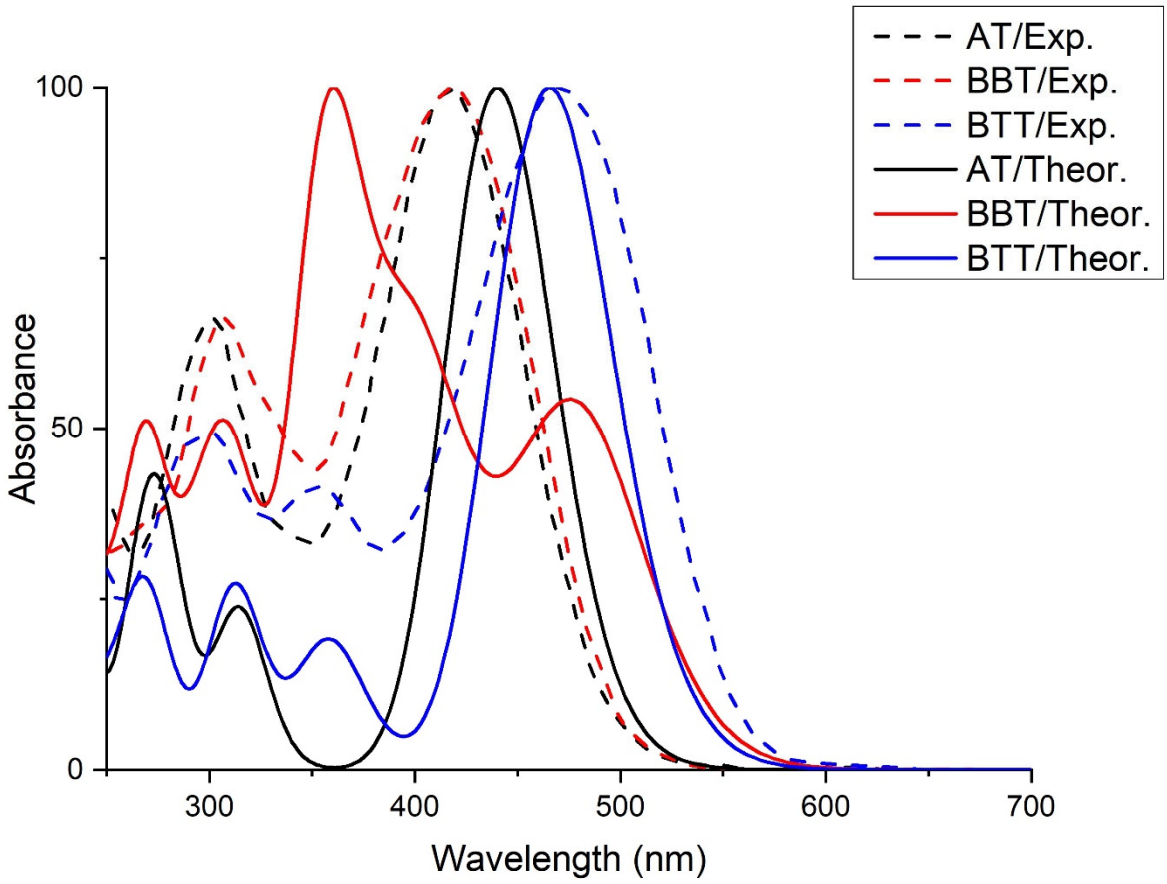

Figure S1. Comparison of UV–Vis absorption spectra of triphenylamine-based dyes. Experimental λmax was taken from the bibliography and theoretical results obtained with TD-DFT and M06-2X/6-31G(d) level of theory.

The experimental values were added with the permission of the authors, adding the citation of the bibliography. For a better appreciation of the results, these were normalized.

Table S1. Stokes shift of triphenylamine based dyes at M06-2X/6-31G(d) level of theory.

Molecule	Stokes Shift (nm)
AT	66
TPAZ1	-
TPAZ2	70
BBT	82
TPAZ3	159
TPAZ4	164
TPAZ5	194
BTT	72
TPAZ6	102
TPAZ7	104

* TPAZ1 does not present emission.