Back to the future: asymmetrical DπA 2,2'-bipyridine ligands for homoleptic copper(I)-based dyes in dye-sensitized solar cells

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Metal complexes used as sensitizers in dye-sensitized solar cells (DSCs) are conventionally constructed using a push-pull strategy with electron-releasing and electron-withdrawing (anchoring) ligands. In a new paradigm we have designed new D π A ligands incorporating diarylaminophenyl donor substituents and phosphonic acid anchoring groups. These new ligands function as organic dyes. For two separate classes of D π A ligands with 2,2'-bipyridine metal-binding domains, the DSCs containing the copper(I) complexes [Cu(D π A) 2] + perform better than the push-pull analogues [Cu(D D)(AA)] + . Furthermore, we have shown for the first time that the complexes [Cu(D π A) 2] + perform better than the organic D π A dye in DSCs. The synthetic studies and the device performances are rationalised with the aid of density functional theory (DFT) and time-dependent DFT (TD-DFT) studies.
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