Design of new redox active copper complexes-based electrolytes for dye sensitized solar cells.

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Organometallic complexes have shown to be promising alternative to the conventional and state of the art iodide/triiodide redox couple. Such compounds offer attractive features over the traditional iodide couple, such as faster one electron transfers following Marcus Theory, low extinction coefficient and the possibility to fine tune the redox potential as well as kinetics through the rational design and synthetic modification of new ligands.

At first, octahedral cobalt based complexes were studied and they proved to be very well compatible with organic dye, producing outstanding results in DSSCs^[1]. However, the high reorganizational energy required for the spin change between the two oxidation states, was limiting their performances.

On the other hand, copper complexes do not present such limitations and by choosing the ligand that would optimize the geometry of the reduced and oxidized parameter one can aim to significantly reduce the energy losses due to the redox process^[2]. The first report of copper based electrolytes in DSSCs rose 10 years ago. Three copper complexes were used as redox mediators in a dye sensitized solar cell along with Ruthenium dye N719 and produced PECs ranging from 0.12% to 1.4%^[3]. Few years later the number were increased to 7% with the N3 dye^[4] and pushed to 10% with the organic dye Y123^[5].

Copper ions have high affinity with nitrogen based ligands and especially bidentate ligands such as 2,2' bipyridine or 1,10-phenanthroline derivatives. The geometry and electronic properties can be finely tuned by introducing bulky, electron rich or electron deficient functionalities on the aromatic ring of the pyridine.

In this regard, we herein present the synthesis of new copper complexes and their electrochemical characterization as well as device performances in dye sensitized solar cells.

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