

Influence of Anchoring Group Location in Ru-based Polypyridyl Sensitizers on the HOMO/LUMO Gap and Total Solar-to-electric Conversion Efficiency for Dye-sensitized Solar Cells

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Introduction

- Dye-sensitized solar cells (DSSCs) show promise as photovoltaic devices which can be made of low cost non-toxic materials with simple manufacturing processes and have the capability to last long enough in the performance environment to provide sufficient return on investment.
- Installation of DSSCs with an efficiency of 10% on about 0.1% of the earth's surface area would be enough to satisfy our current energy needs of 15 TW/annum [1, 2].
- Current research DSSCs have exceeded efficiencies of 11% [3] large module efficiencies have surpassed 10% [4].
- Our objective is to develop efficient sensitizers for DSSCs to improve cell efficiencies and facilitate commercialization.

Operating Principles

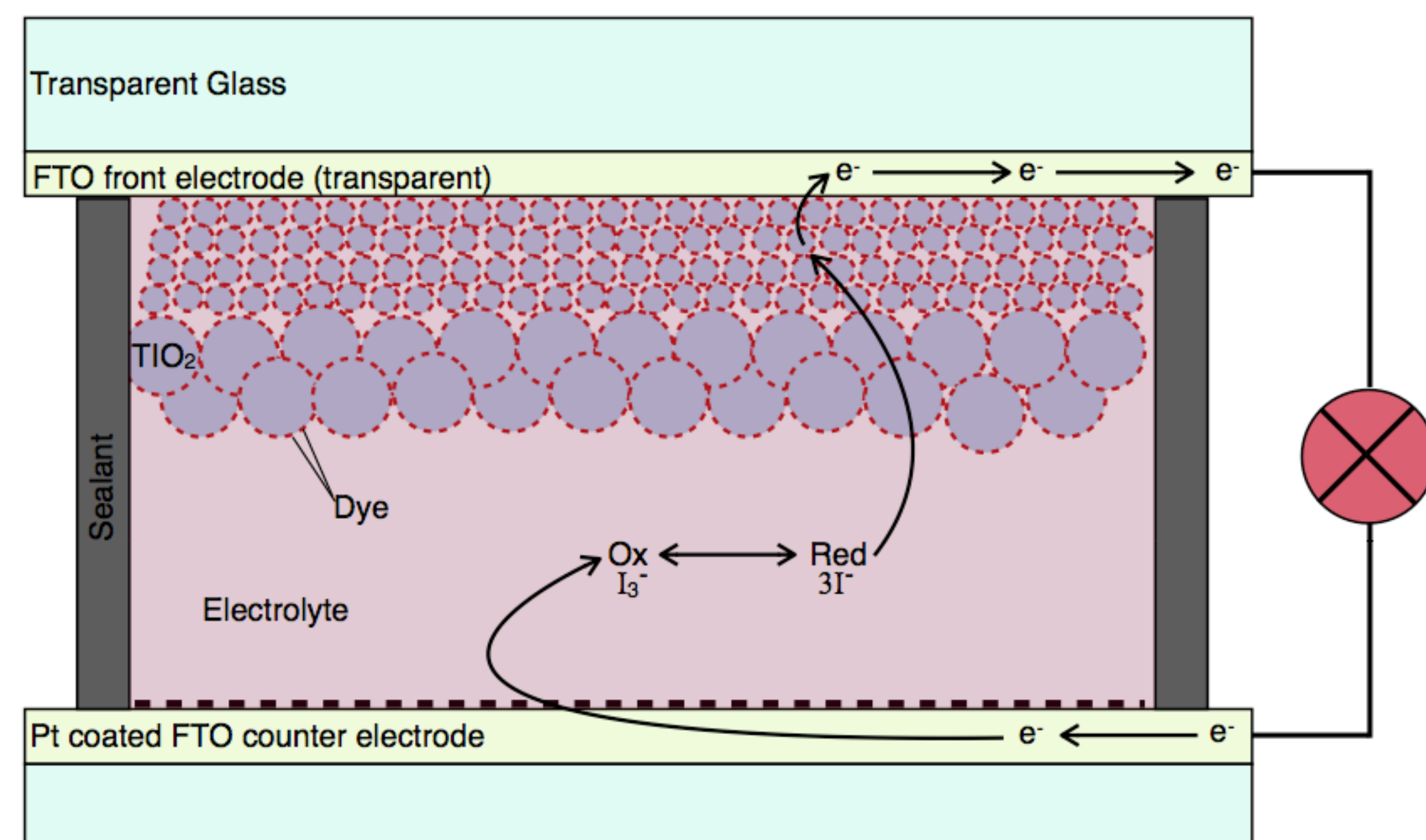
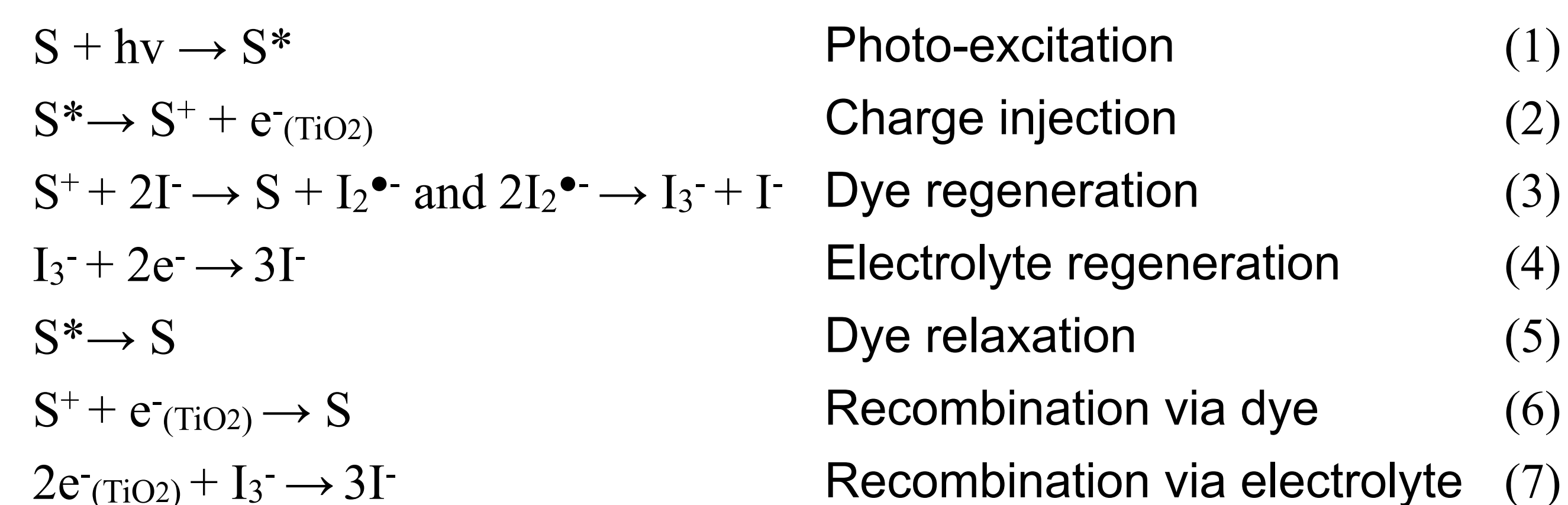


Figure 1: Schematic of dye-sensitized solar cell components.

- Equations 1 through 7 define the processes that take place in DSSCs upon exposure to light.



Experimental

- Two novel Ru-based dyes were with isomeric structures were synthesized and purified.

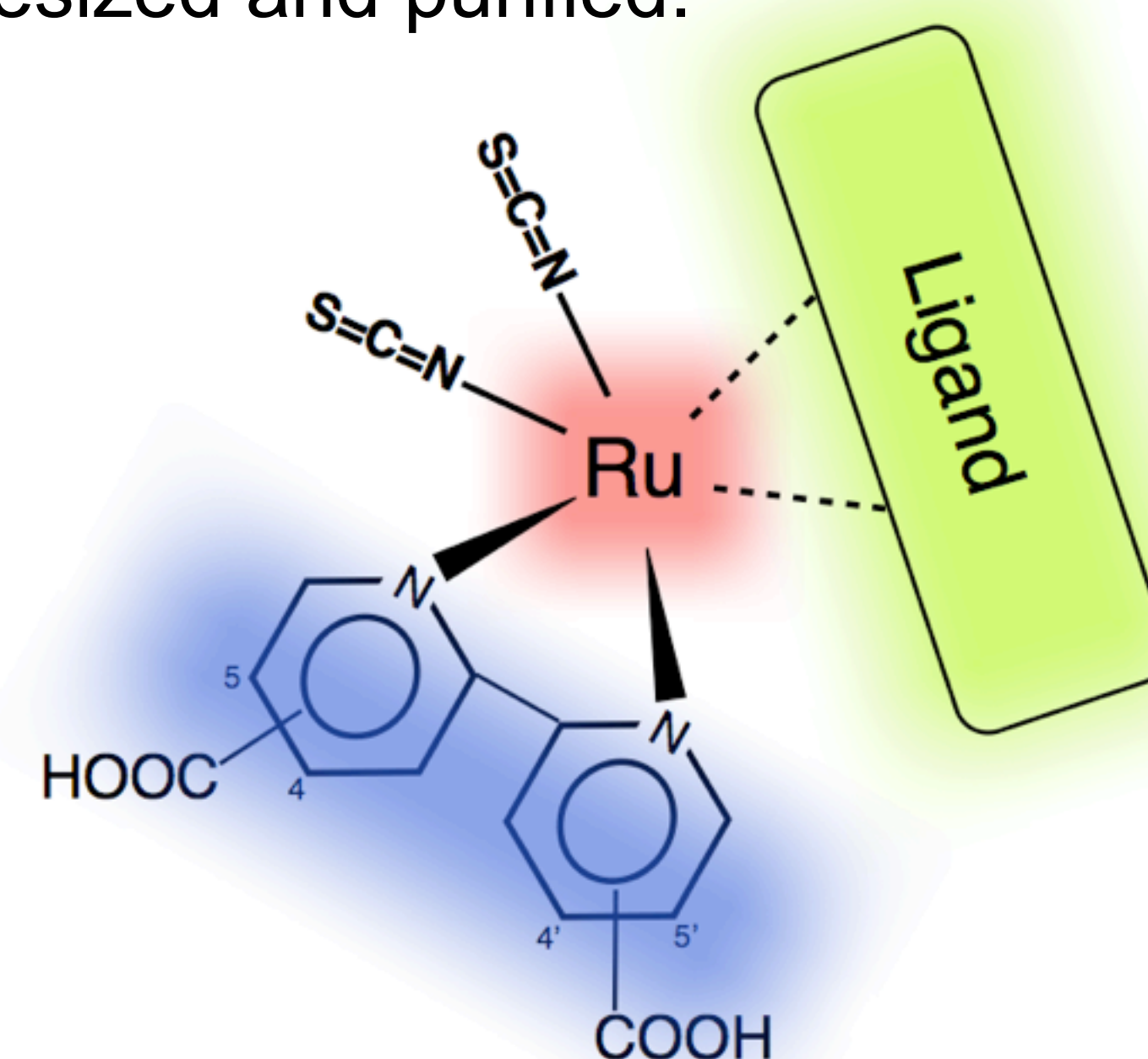


Figure 2: Schematic of synthesized dyes. The placement of the carboxylic acid (COOH) anchoring groups 4,4' in RAAP and 5, 5' in RAAM (Structures are proprietary, patent filed at NCSU).

- Total solar to electric conversion and Incident Photon-to-Current Efficiency (IPCE) were measured for isomers RAAP and RAAM, and N-719 sensitizers at the same conditions.
- HOMOs were measured with an AC3 type photoelectron spectrometer (Riken Keiki Co., Ltd.) and LUMOs were calculated from visible and emission spectrometry.

Results and discussion

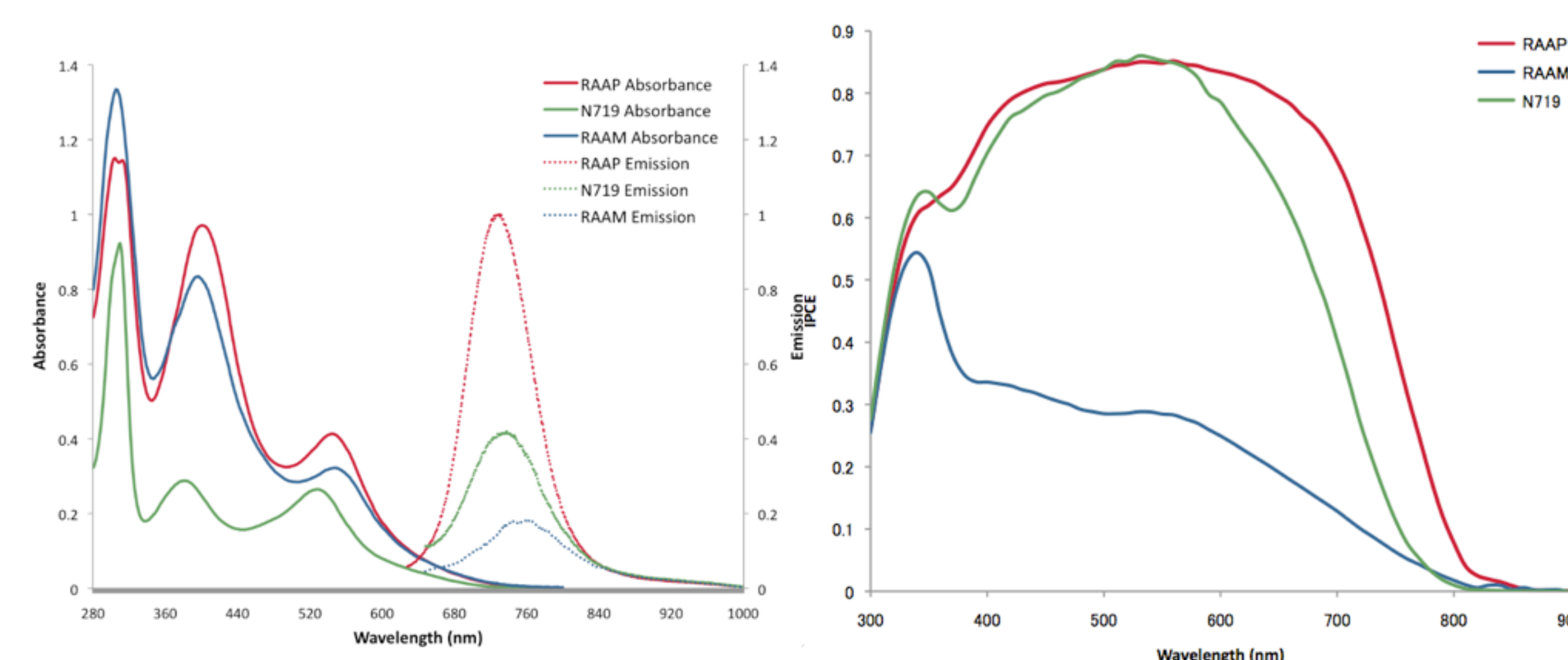


Figure 3: UV-Vis and emission spectra of dyes measured using $2 \times 10^{-5} M$ solutions in DMF (left) and photo-action spectra of sealed DSC's (right).

- Both novel complexes are bathochromically shifted with much greater extinction coefficients than the benchmark dye N-719.

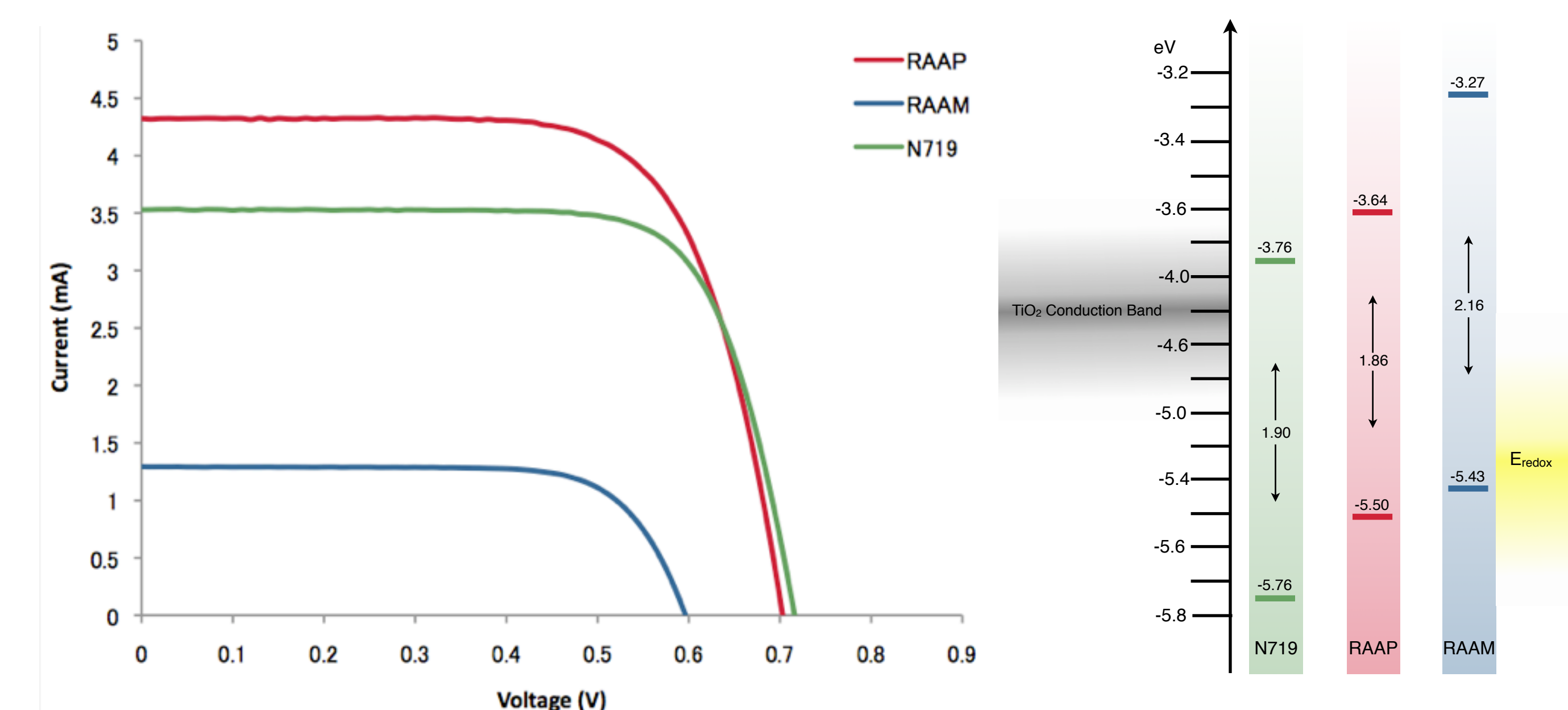


Figure 4: IV curves (left) and schematic showing HOMO, LUMO and band-gap of N719 and novel complexes (right).

Table 1: IV characteristics of DSC's

Sensitizer	J_{sc} (mA/cm ²)	V_{oc} (V)	Fill Factor	Efficiency (%)
N719	15.3	0.716	0.741	8.131
RAAP	18.8	0.703	0.701	9.240
RAAM	5.62	0.596	0.734	2.459

- RAAP produced more photocurrent at longer wavelengths than N-719.
- The positioning of the HOMO and LUMO in RAAP is optimized for efficient electron injection and dye regeneration via electrolyte.

Conclusions and future work

- RAAP outperformed N-719 under standard testing conditions.
- Optimization of devices based on RAAP should further improve performance of devices.
- TCSPC should be conducted to measure excited state lifetimes for in-depth understanding of subject.
- Development of dyes based on understanding can help develop panchromatic sensitizers.

References:

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