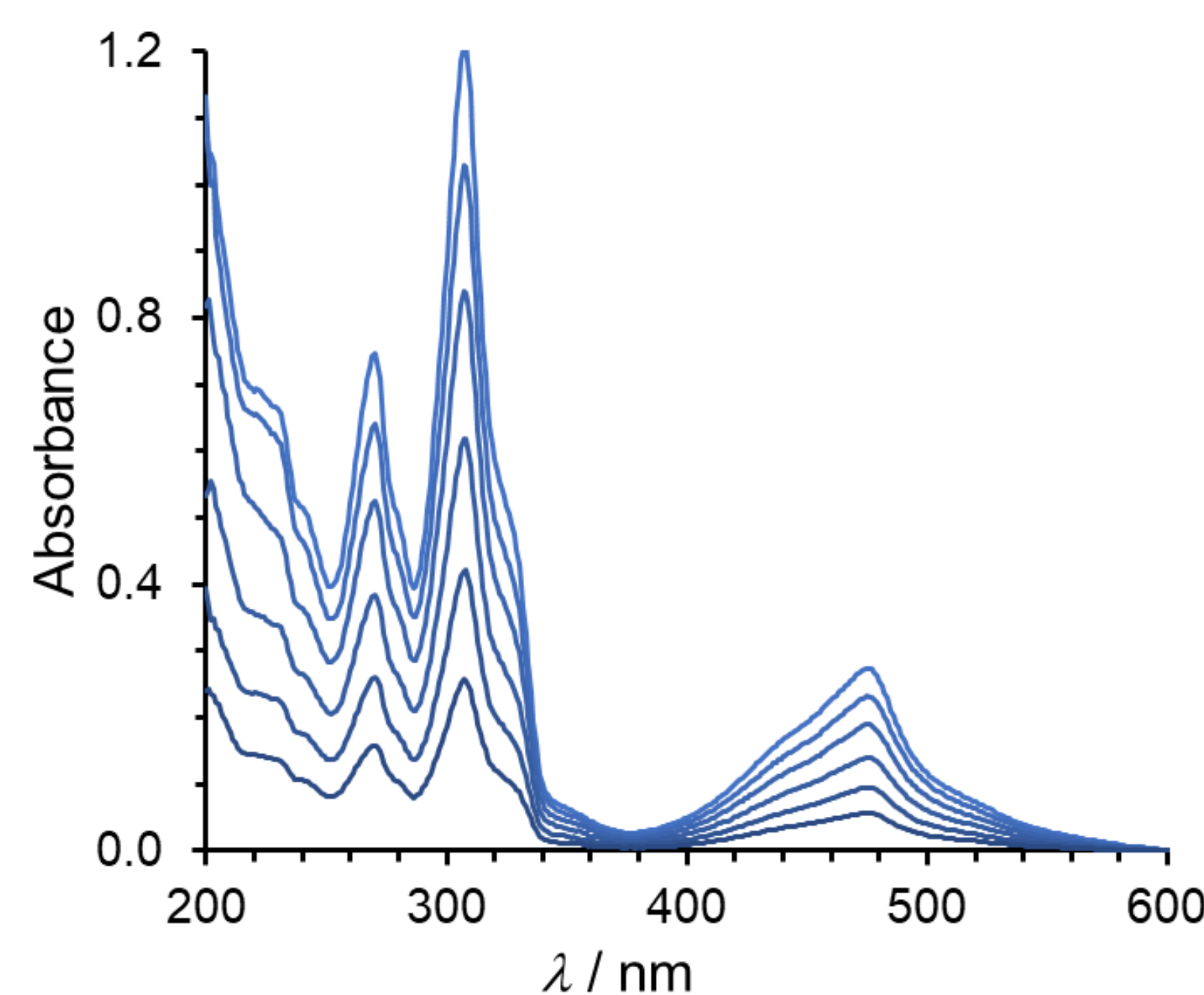


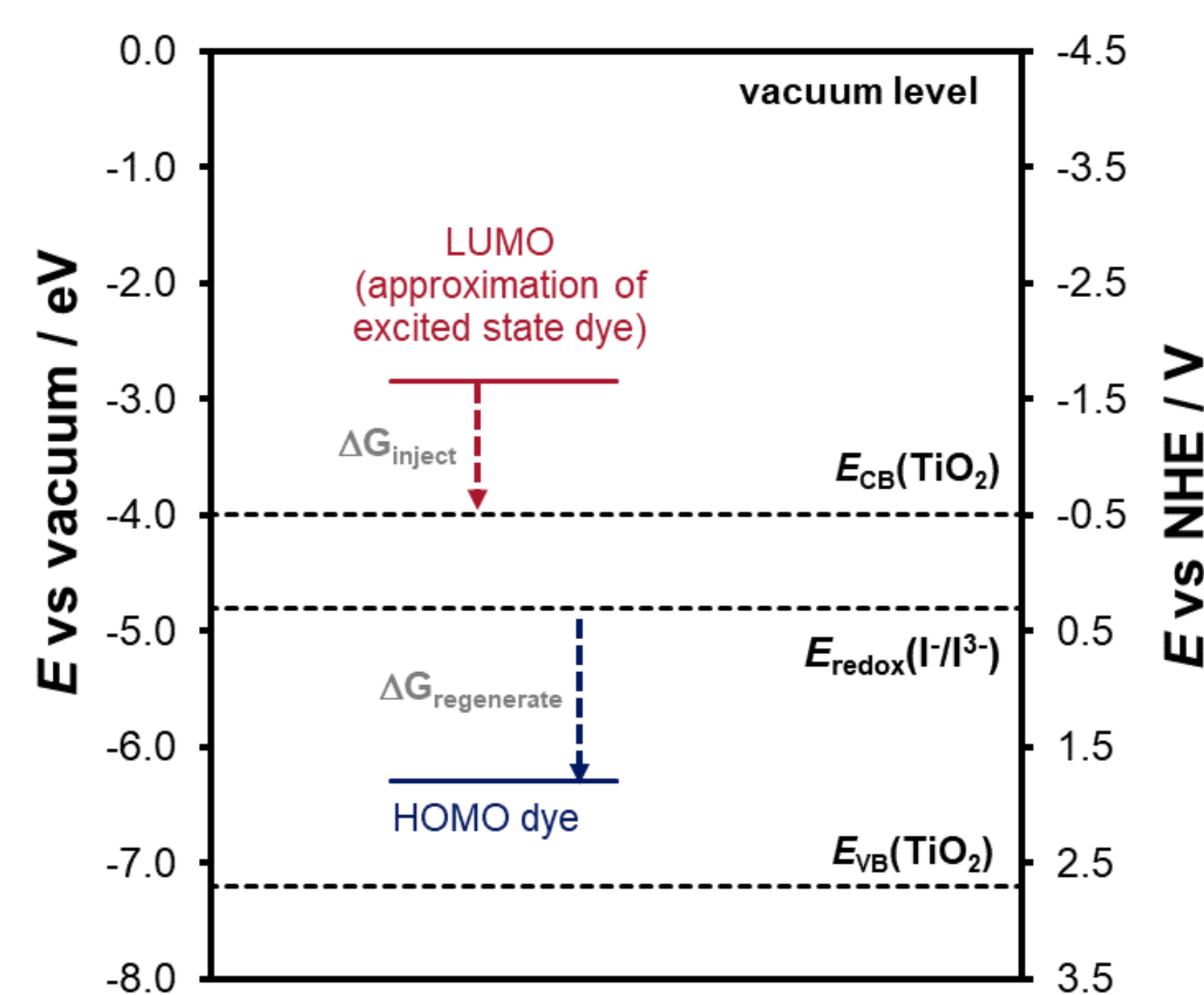
CV and UV of bis(2,2':6',2''-terpyridine)ruthenium – application in dye-sensitized solar cell (DSSC)

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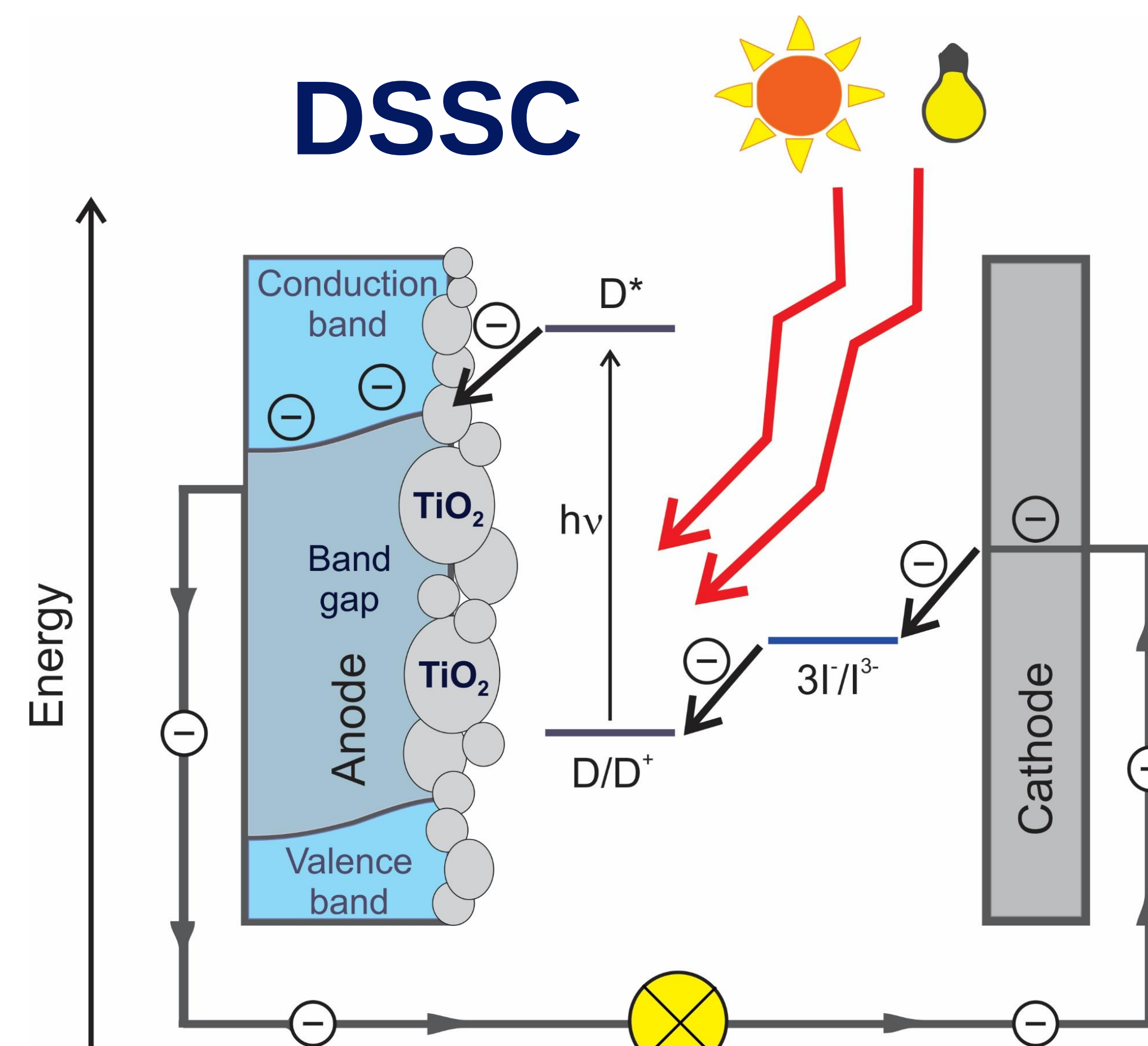
UV-vis



MO energies



DSSC

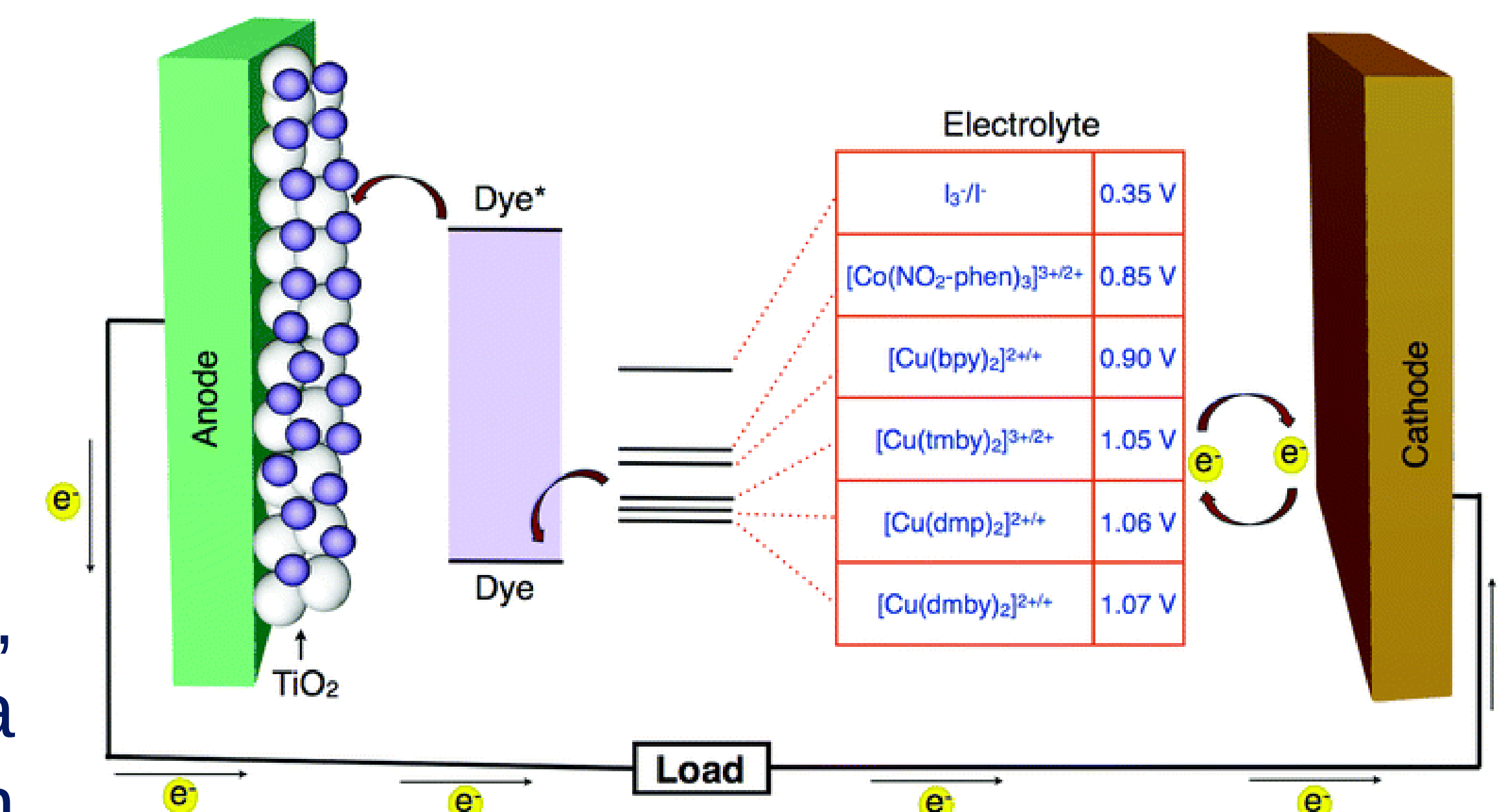


Basic operation of a DSSC:

(i) absorption of sunlight by the dye D, (ii) injection of excited electrons into a TiO_2 semiconductor, (iii) electron transport through the semiconductor, (iv) regeneration of the dye molecule by the I_3^-/I^- redox electrolyte, and (v) collection of electrons at the electrode to generate an electric current.

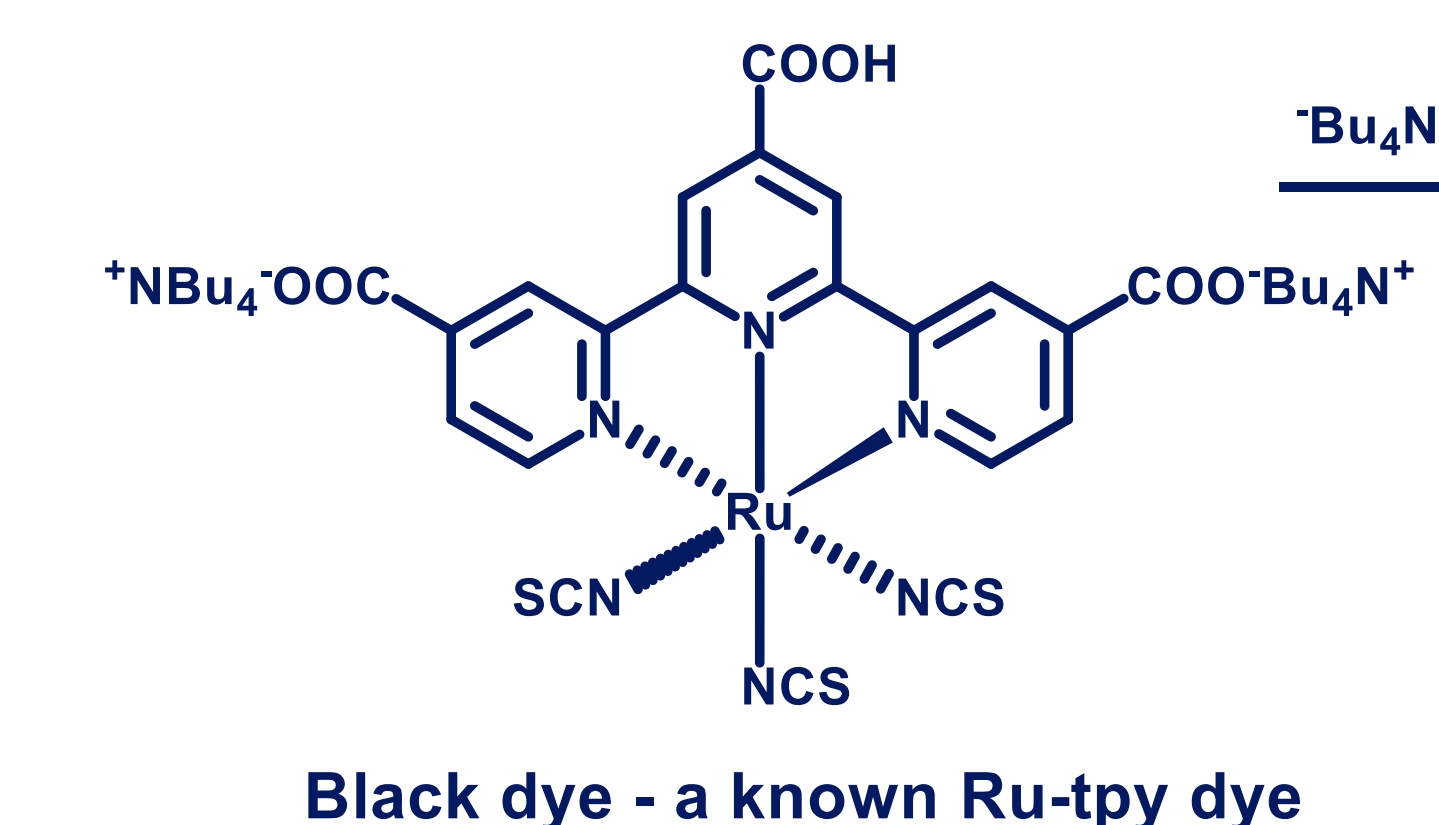
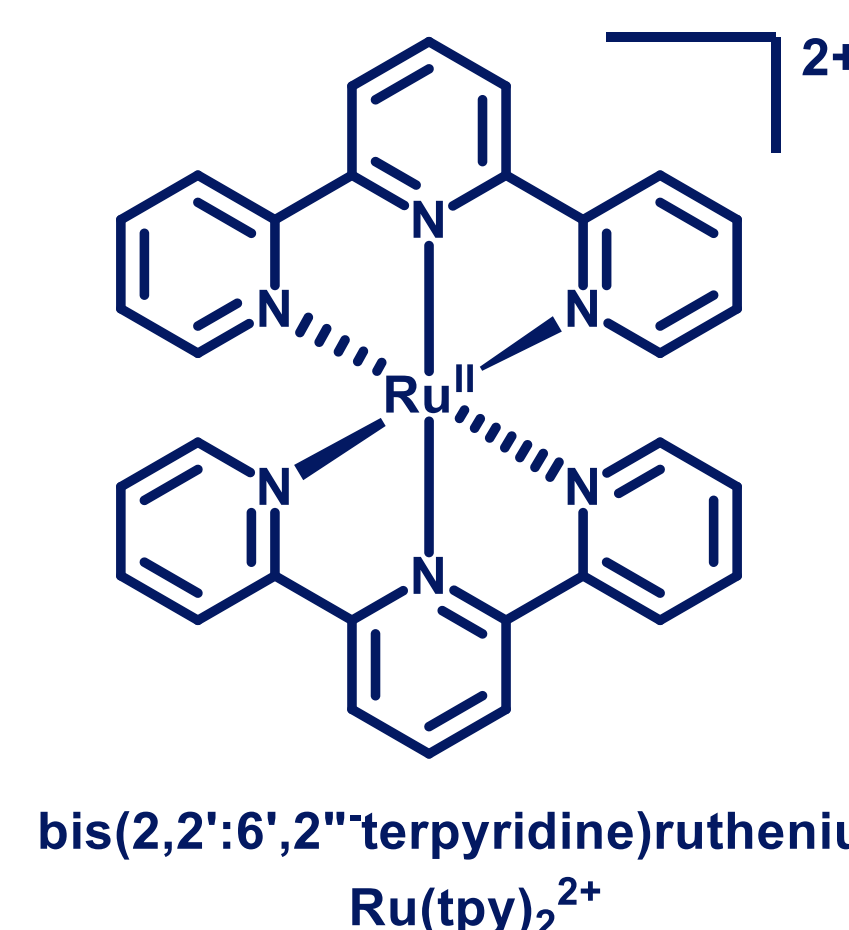
Reprinted from Journal of Molecular Graphics and Modelling, 121, J Conradie, DFT study of UV-vis-properties of thiophene-containing $\text{Cu}(\beta\text{-diketonato})_2$ – Application for DSSC, 108459, 2023, with permission from Elsevier

Redox energies

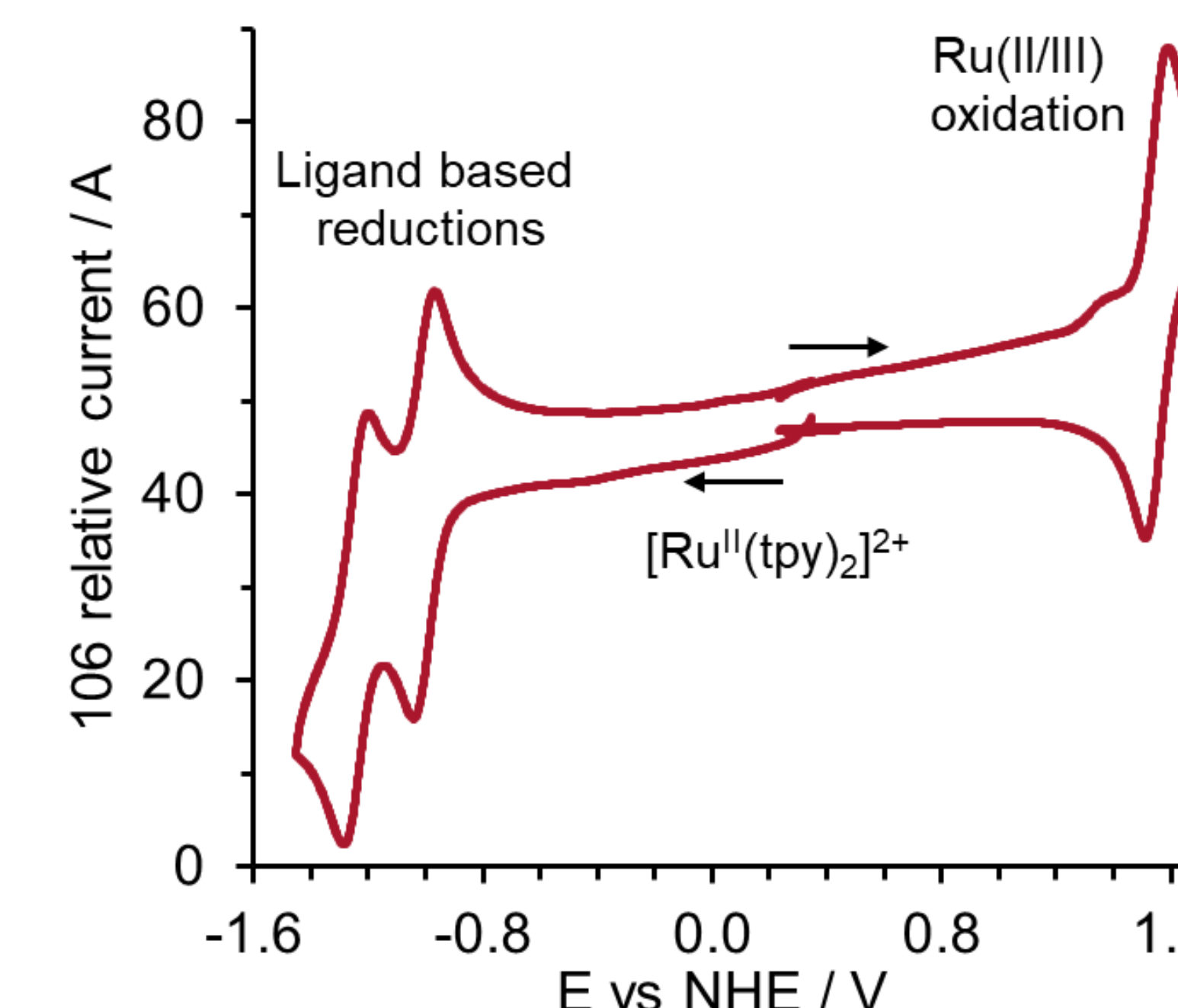


Schematic energy level diagram of a DSSC, showing redox energies of electrolytes vs NHE

From Mater. Adv. 2 (2021) 1229–1247 (Open Access)



CV



Cyclic voltammogram (CV) of $\text{Ru}(\text{tpy})_2$ in CH_3CN at 0.100 Vs^{-1} .

Data from N.G.S Mateyise, M.M Conradie, J Conradie, J. Electroanal. Chem. 2023 DOI: 10.1016/j.jelechem.2023.117807

Application as a dye sensitizer:

- The sun's spectrum peaks at a wavelength of approximately 500 nm.
- The UV-vis spectrum of $\text{Ru}(\text{tpy})_2$, which exhibits a peak in the visible spectrum around 500 nm, is ideal for the absorption of sunlight, a requirement for a dye sensitizer in DSSCs.
- The DFT-calculated HOMO and LUMO energies of $\text{Ru}(\text{tpy})_2$ are favorable, making it a potential candidate for use as a dye in DSSCs.

Application as a redox mediator:

- The range for redox mediators in DSSC with TiO_2 photoelectrode is ca 0.3–1 V versus NHE, depending on the properties of the dye.
- CV of $\text{Ru}(\text{tpy})_2$ indicates that the $\text{Ru}(\text{II/III})$ redox potential is too high to be considered as redox mediator (electrolyte) in a DSSC.