Thieno[3,2-*b*]indole Based Organic Dyes for Efficient Dye-Sensitized Solar Cells

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Dye-Sensitized Solar Cells (DSSCs):

Low cost and efficient devices for the conversion of sunlight into electricity

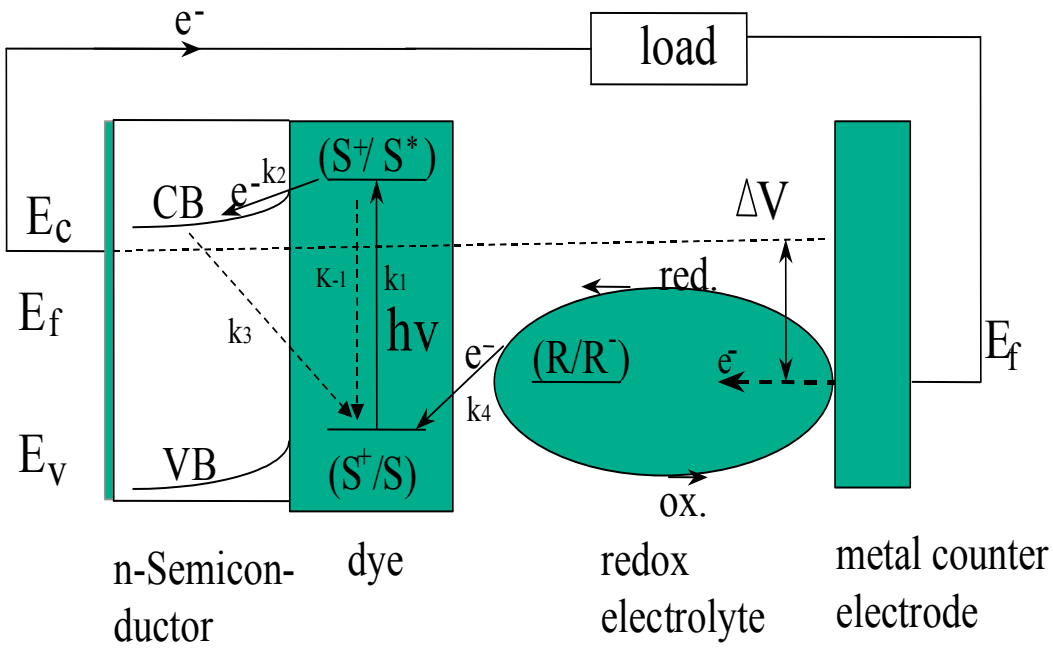
Main processes in DSSCs:

$Dye + h\nu \rightarrow Dye^*$

$Dye^* \rightarrow Dye^+ + e^-(TiO_2)$

$2e^- + 3I_3^- \rightarrow 3I^-$

$3I^- + 2Dye^+ \rightarrow I_3^- + 2Dye$



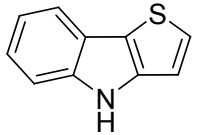
Dye-Sensitized Solar Cells

Design of the organic dyes:

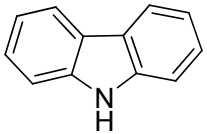
Electron donor: thieno[3,2-*b*]indole moiety *vs.* carbazole moiety

π-conjugated bridge: *n*-hexyl-substituted oligothiophene units

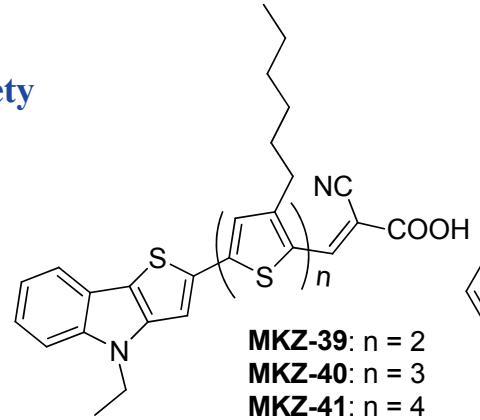
Electron acceptor: cyanoacrylic acid group



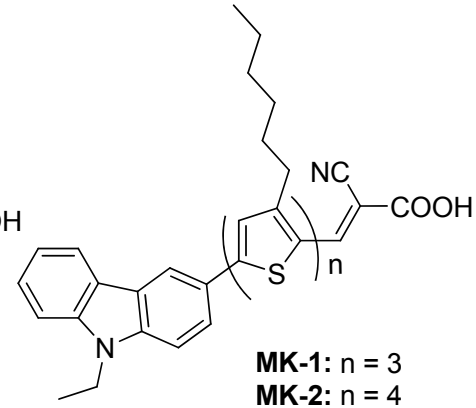
4*H*-thieno[3,2-*b*]indole



9*H*-carbazole

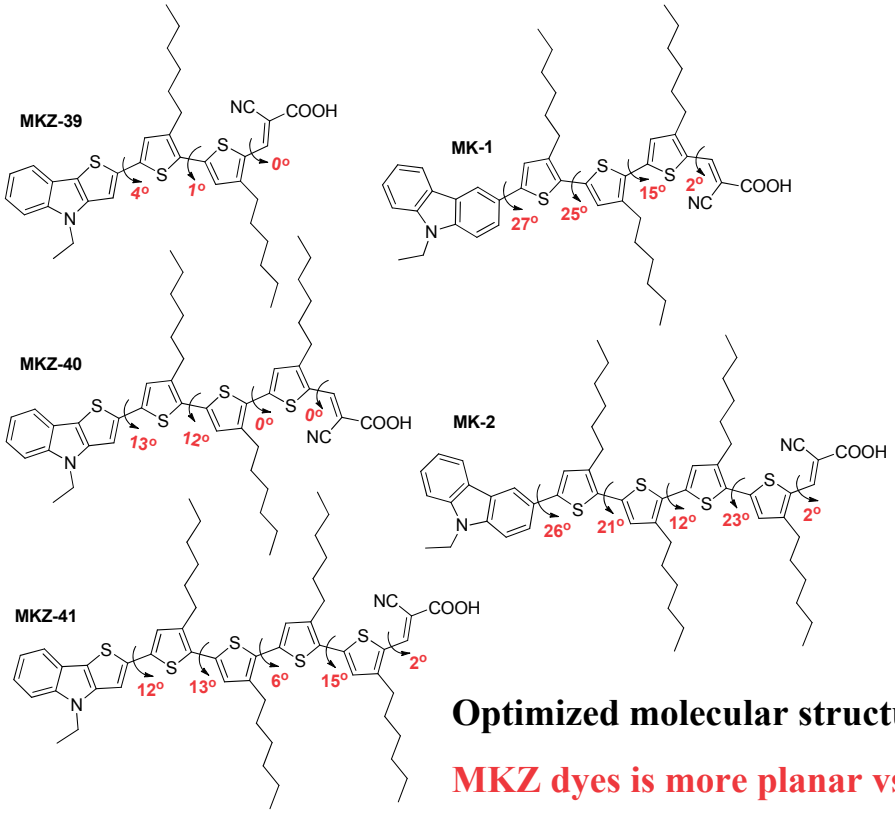


MKZ-39: n = 2
MKZ-40: n = 3
MKZ-41: n = 4



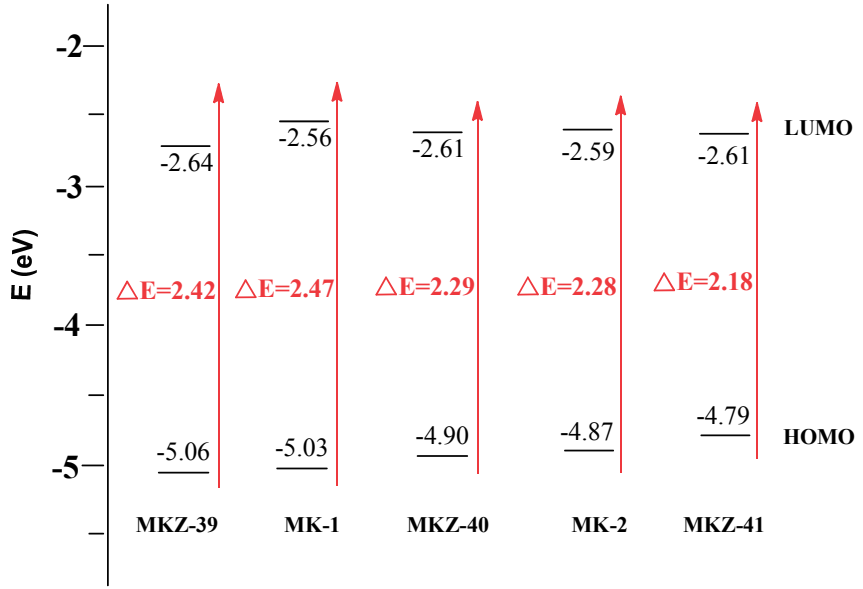
MK-1: n = 3
MK-2: n = 4

Calculations:



Optimized molecular structure

MKZ dyes is more planar vs. MK dyes

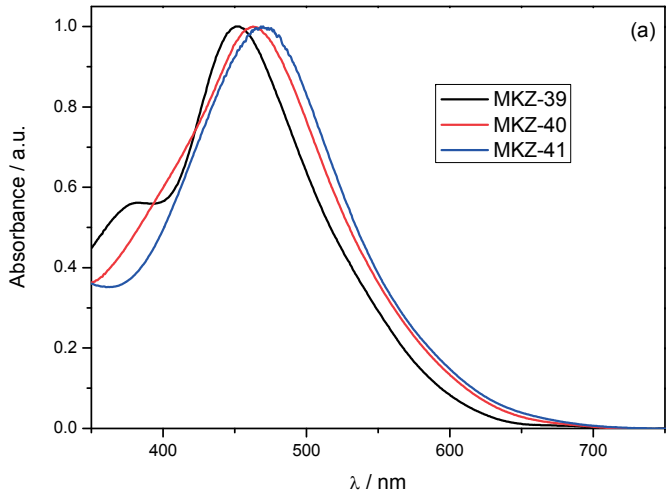


Calculated molecular orbital energy diagram

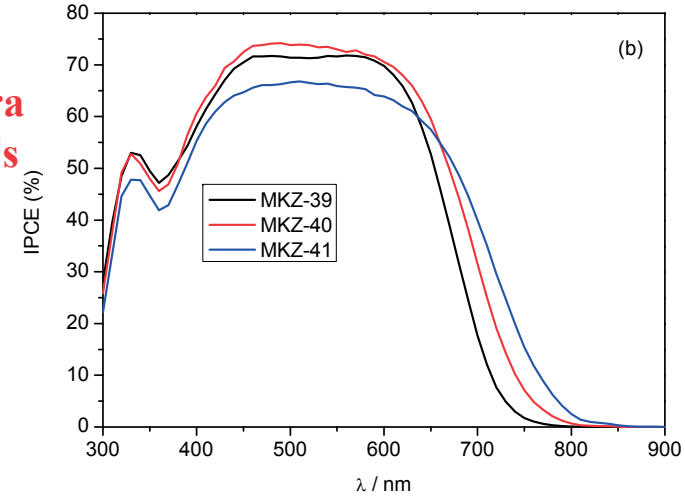
Electron donating ability:

thieno[3,2-*b*]indole moiety > carbazole moiety

(a): Absorption spectra on TiO_2 film



(b): IPCE spectra of the DSSCs

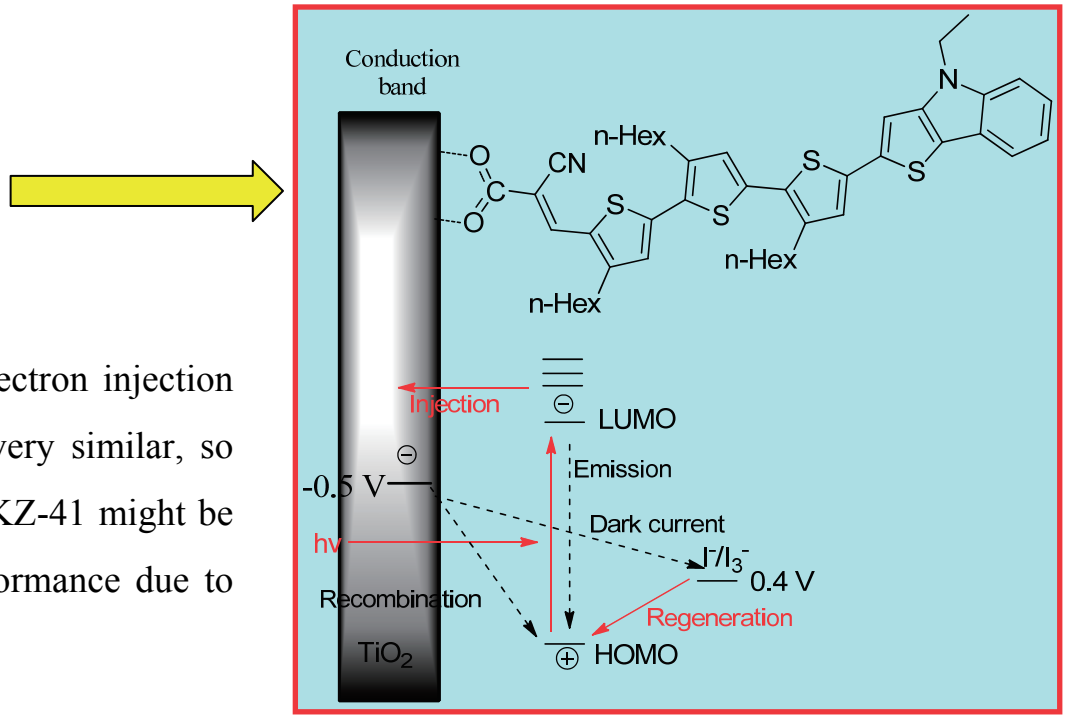


Photophysical, electrochemical and photoelectrochemical properties of the dyes

	λ_{max} / nm (ε / 10^4 M^{-1} cm^{-1})	λ_{max} / nm (on TiO_2 film)	E_{ox}/V (*vs* NHE)	$E_{0\text{-}0}$/eV	E_{ox}*/V (*vs* NHE)
MKZ-39	502 (4.3)	451	1.01	1.97 (630 nm)	-0.96
MKZ-40	496 (4.5)	458	0.89	1.89 (655 nm)	-1.00
MKZ-41	490 (4.6)	466	0.83	1.84 (674 nm)	-1.01

	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF	η (%)
MKZ-39	13.8	0.70	0.77	7.4
MKZ-40	14.6	0.70	0.76	7.8
MKZ-41	15.0	0.66	0.74	7.3

Schematic energy diagram for a DSSC based on MKZ-40, a nanocrystalline TiO_2 electrode, and the I^-/I_3^- redox couple.



Transient absorption spectra indicate that the electron injection efficiency and charge recombination rates are very similar, so smaller driving force for dye regeneration of MKZ-41 might be the main reason for its lower photovoltaic performance due to the increased HOMO energy level.

Conclusions:

◆ Three new organic dyes based on thieno[3,2,-*b*]indole were synthesized and used for DSSCs for the first time, yielding a good performance with 7.8% overall conversion efficiency under standard AM 1.5G irradiation (100 mW cm^{-2}).

◆ In similar donor-π-acceptor structure, the electron donating ability of thieno[3,2-*b*]indole unit is stronger than that of carbazole; using thieno[3,2-*b*]indole as the donor part could hold the dye molecule in a more planar conformation compared with those carbazole based dyes.

◆ The photovoltaic performance of the dyes is dependent strongly on their HOMO energy level, which has much relationship with the regeneration of the dyes.