



**The Abdus Salam
International Centre for Theoretical Physics**



1938-8

Workshop on Nanoscience for Solar Energy Conversion

27 - 29 October 2008

Charge Recombination Studies in Hybrid Molecular Photovoltaic Devices

Emilio PALOMARES
*Institute of Chemical Research of Catalonia
Avinguda Paisos Catalans 16
43007 Tarragona
Spain*



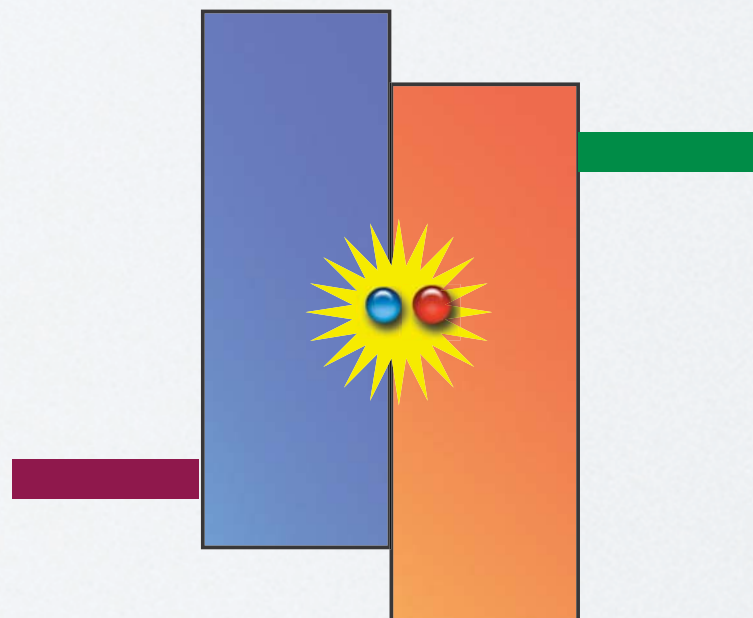
Charge Recombination Dynamics in Molecular Photovoltaic Devices.

Dr. Emilio Palomares. ICREA Research Professor
Institute of Chemical Research of Catalonia (ICIQ).

e-mail: epalomares@iciq.es

Photons in....Electrons Out

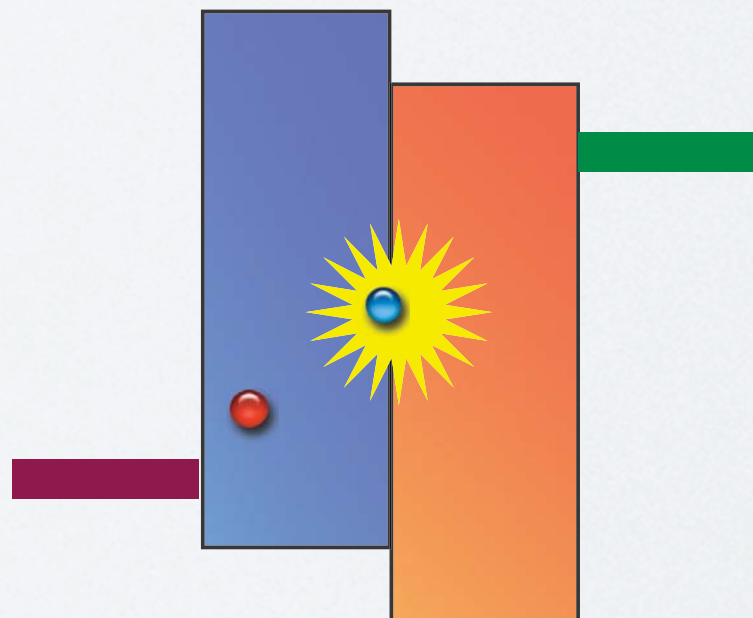
● Always Different Interfaces



Molecular Solar Cells

Photons in....Electrons Out

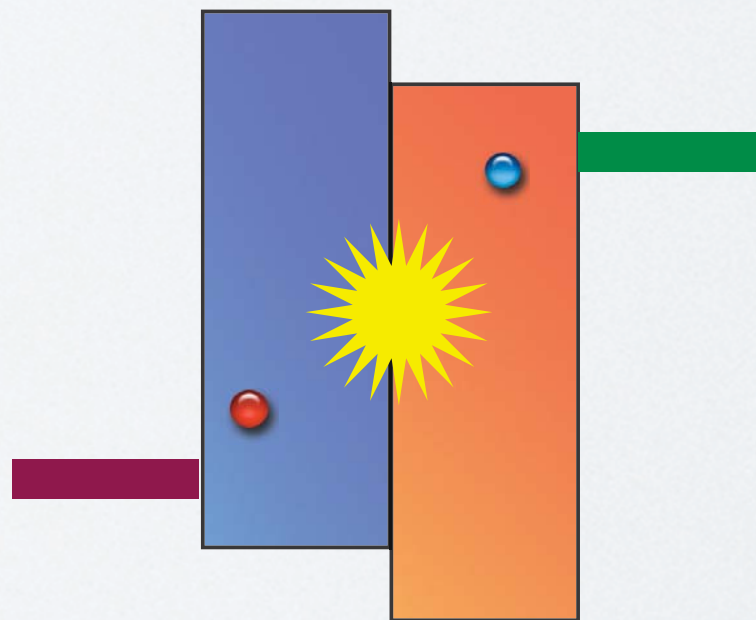
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Molecular Solar Cells

Photons in...Electrons Out

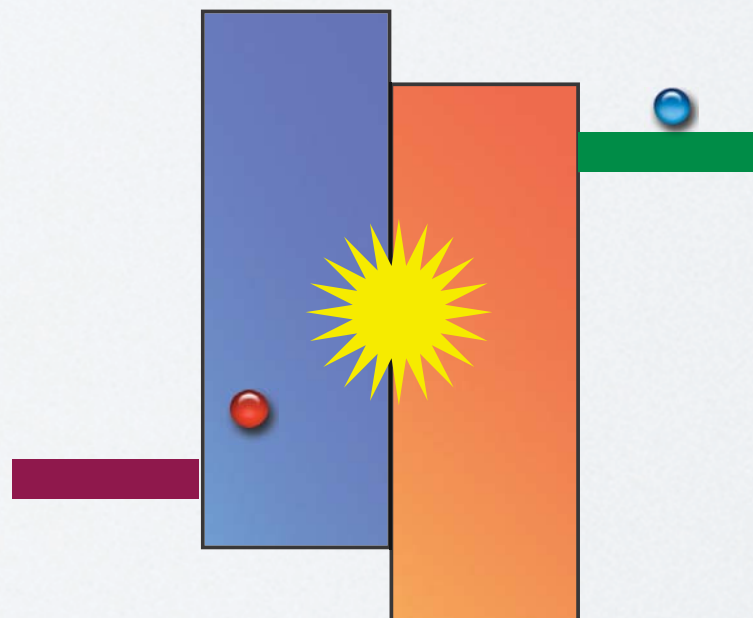
- Always Different Interfaces



Molecular Solar Cells

Photons in....Electrons Out

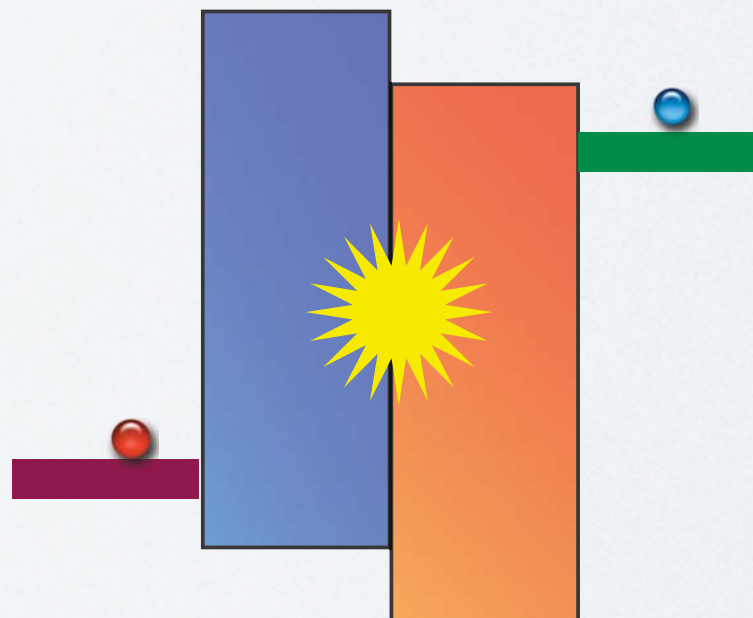
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Molecular Solar Cells

Photons in....Electrons Out

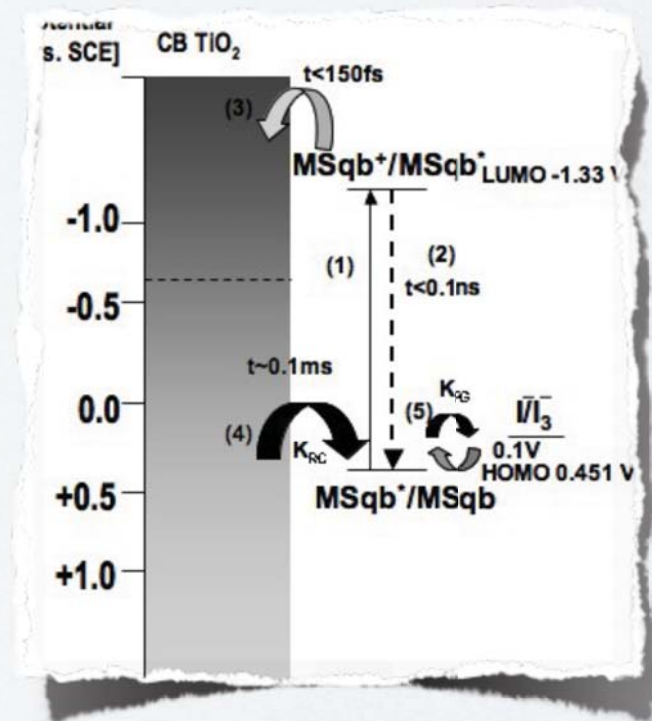
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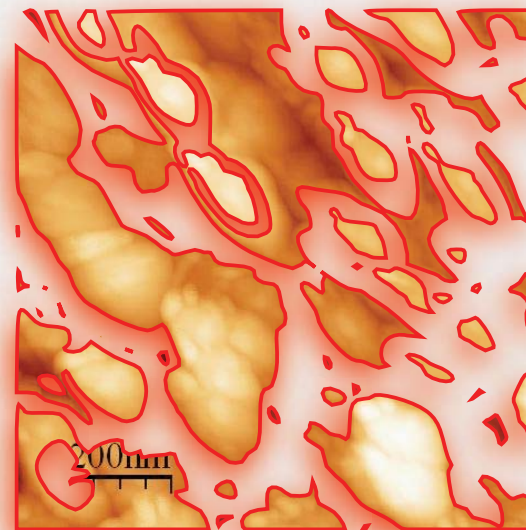
Molecular Solar Cells

Different Photovoltaic Devices

Two different approaches



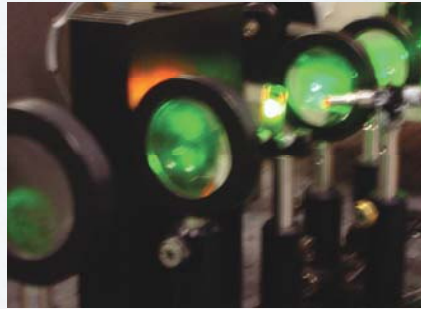
Dye Sensitised
Solar Cells



"Blend" Solar
Cells

Charge Transfer Processes

L-TAS



E_{TiO_2}/DYE Injection



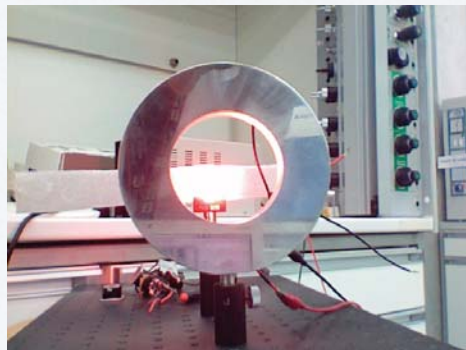
E_{TiO_2}/DYE^+
RECOMBINATION

TCSPC



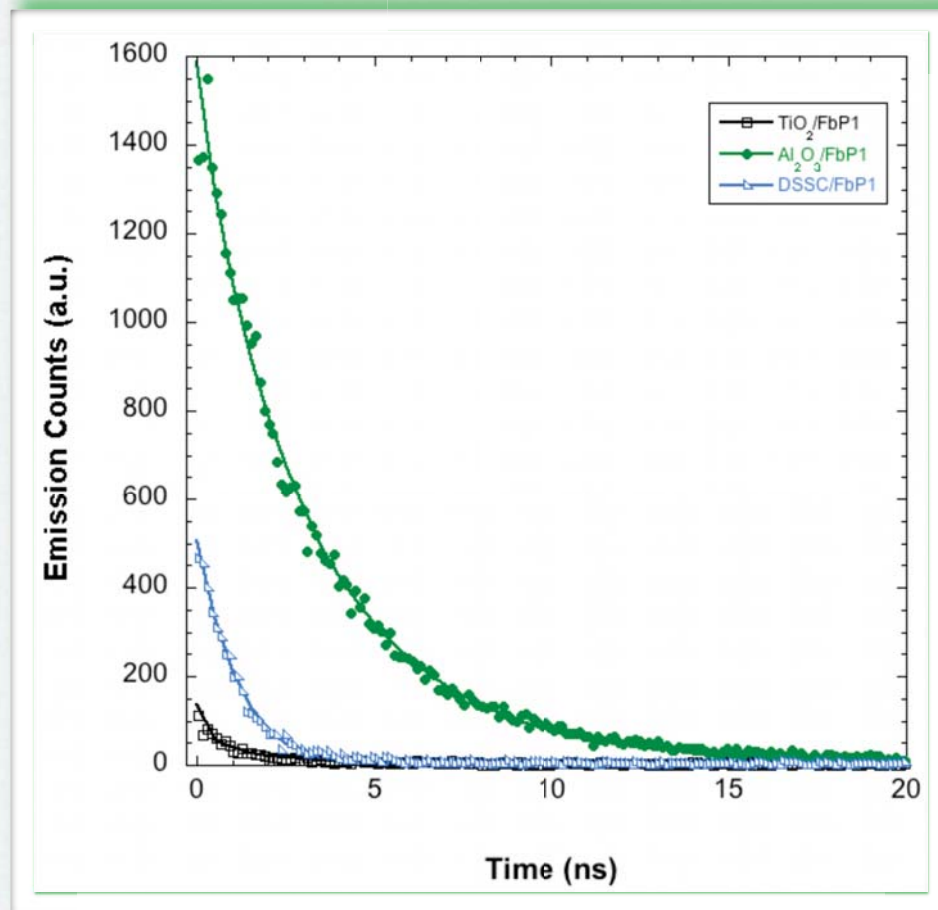
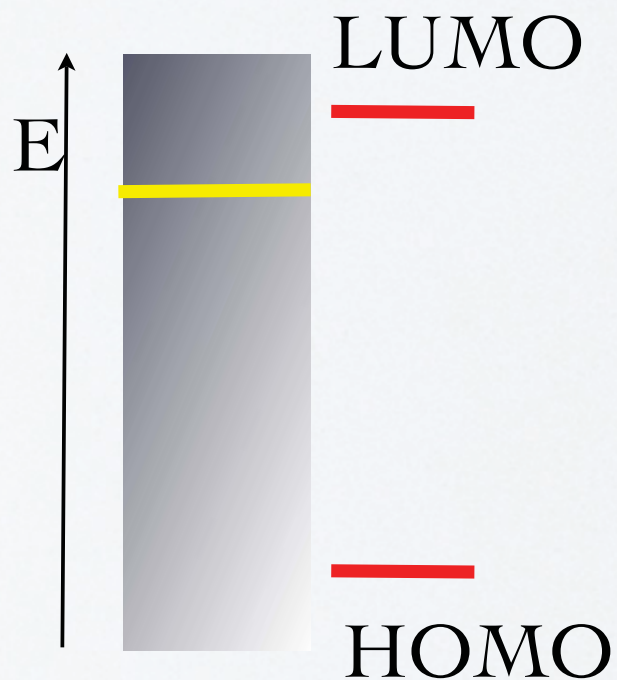
E_{TiO_2}/HTM
RECOMBINATION

TPV



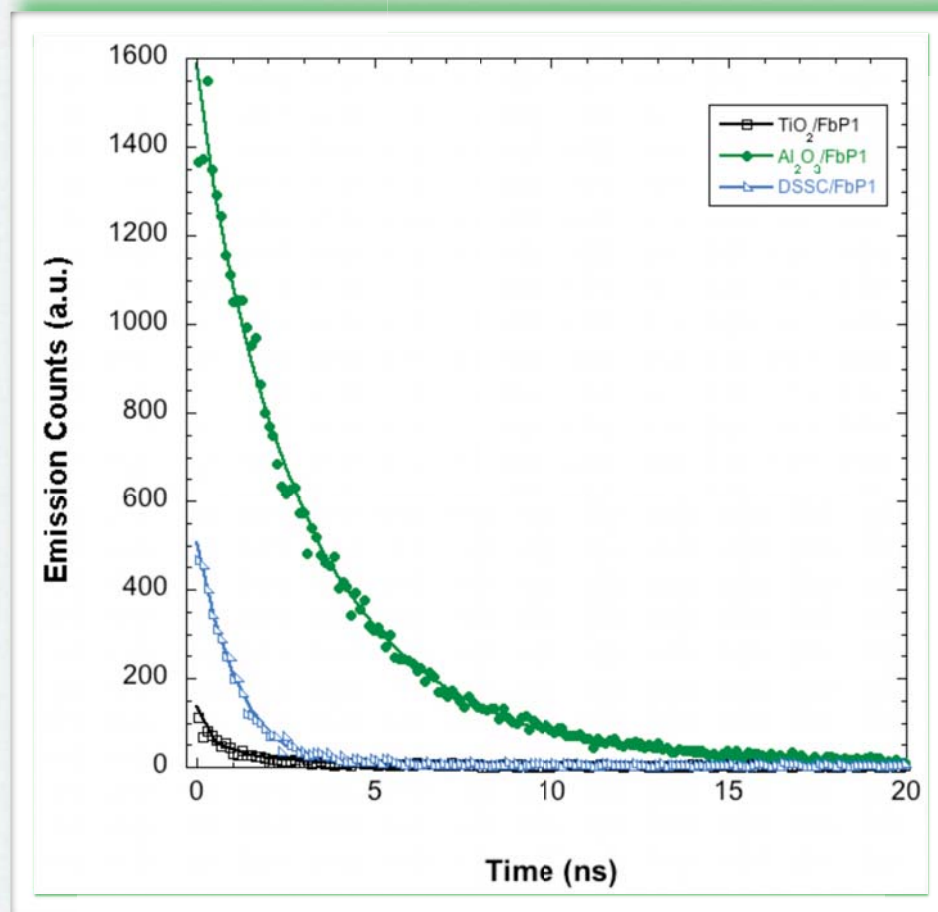
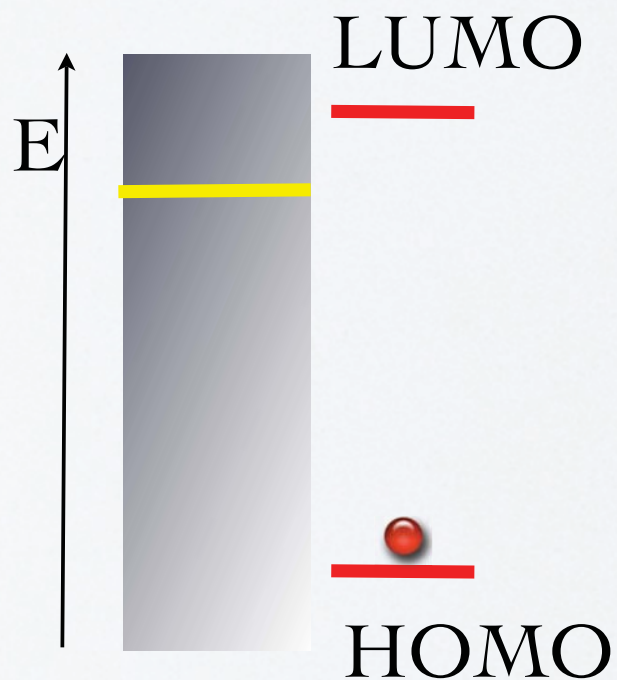
HTM/DYE^+ Regeneration

Charge Transfer Processes



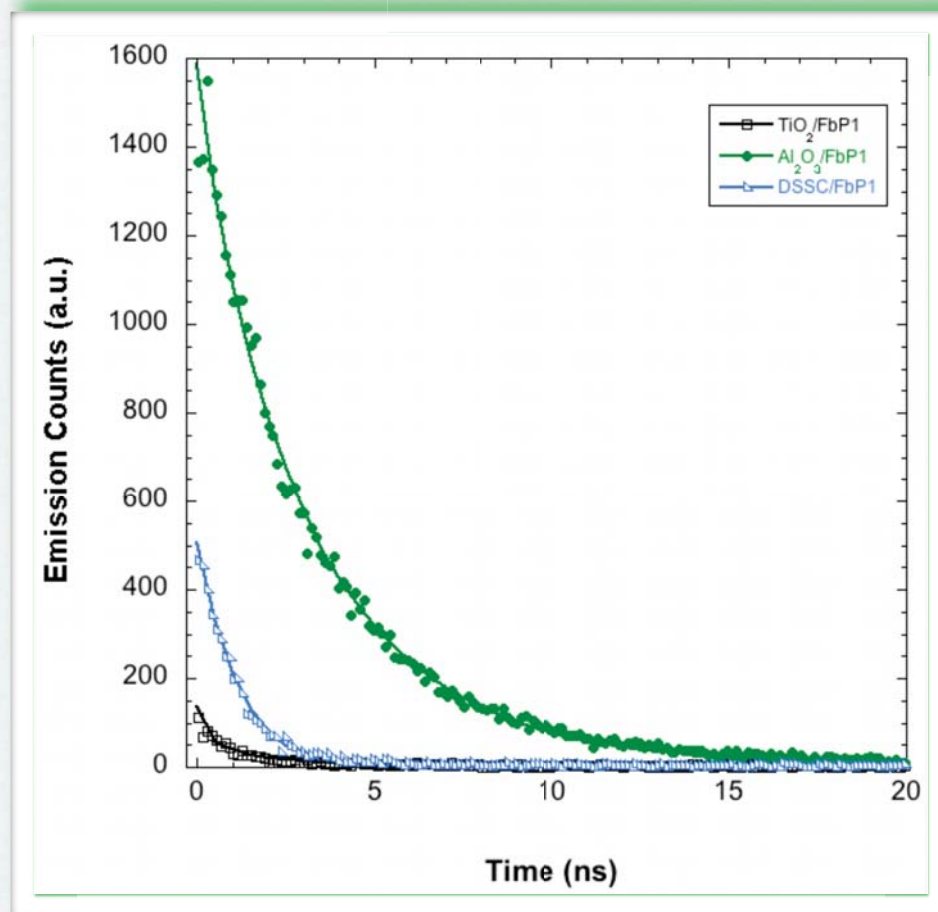
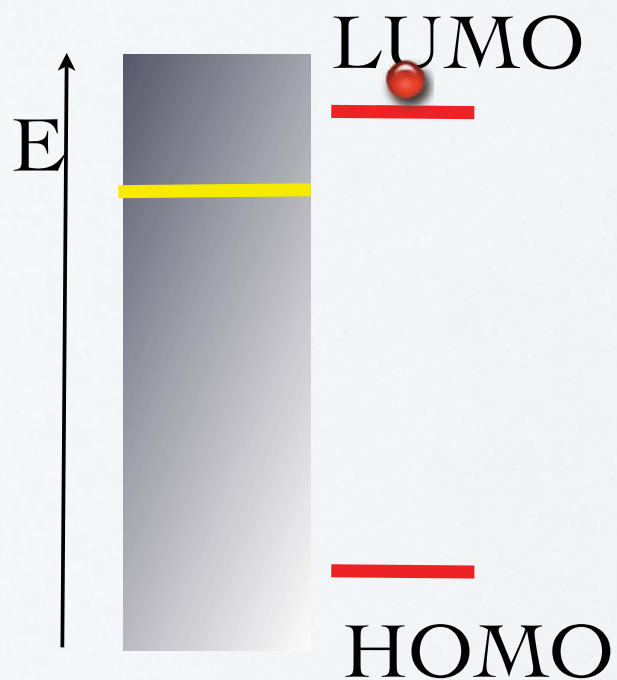
$\text{ETiO}_2/\text{DYE}^+$ injection

Charge Transfer Processes



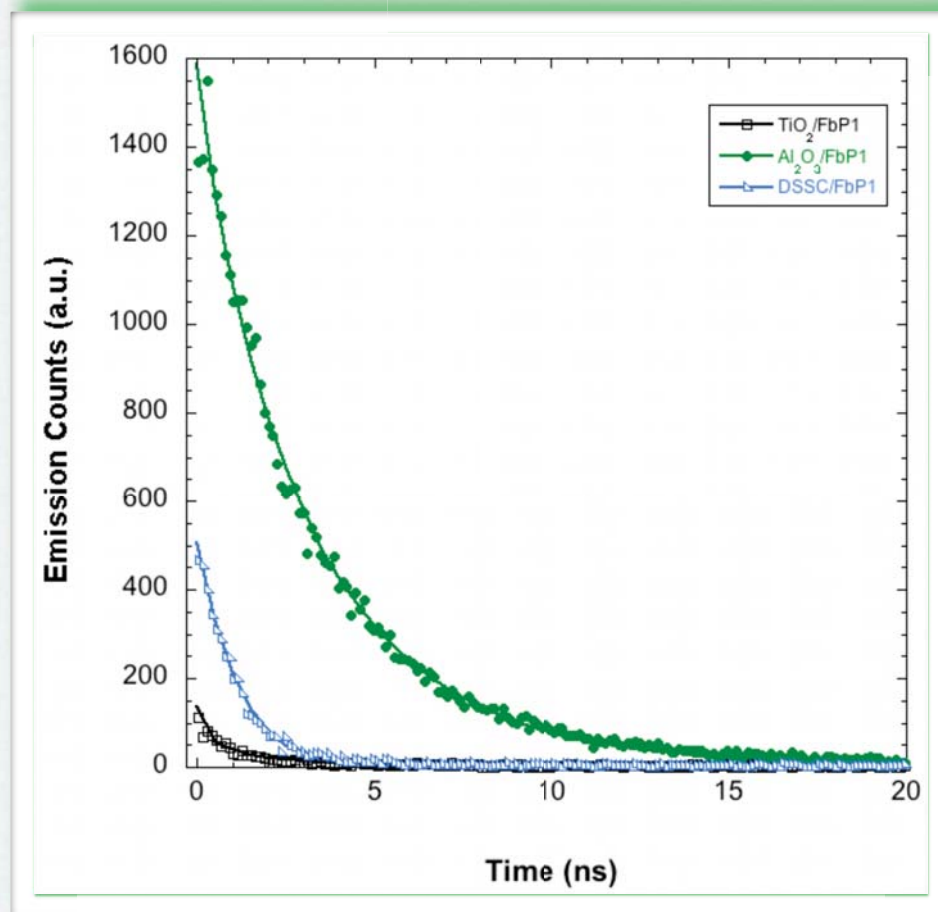
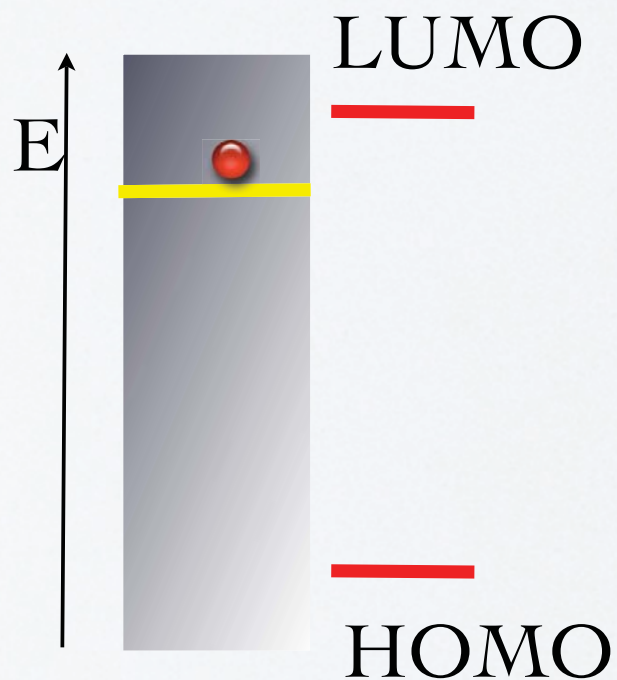
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Charge Transfer Processes



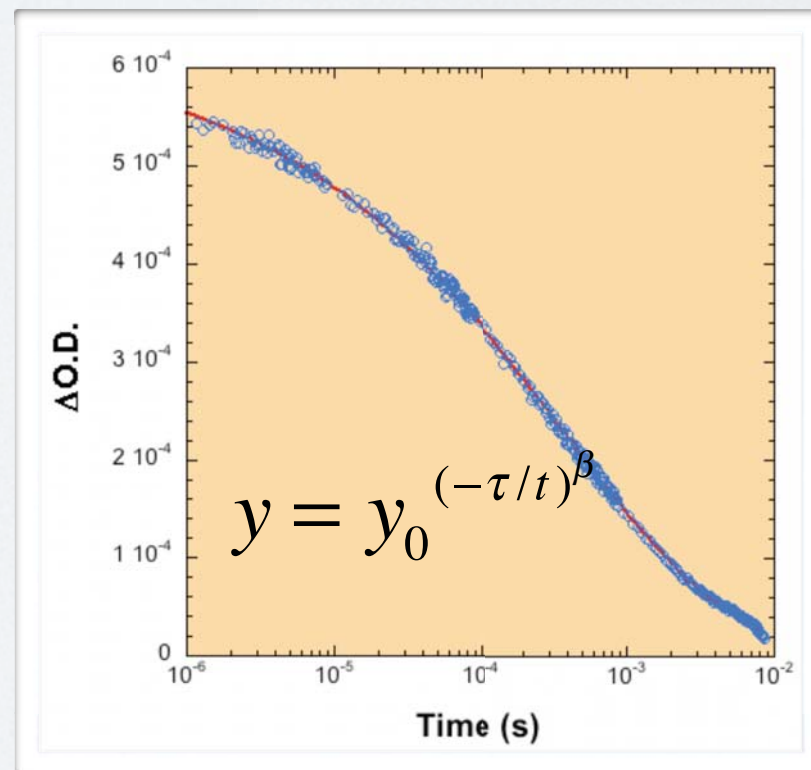
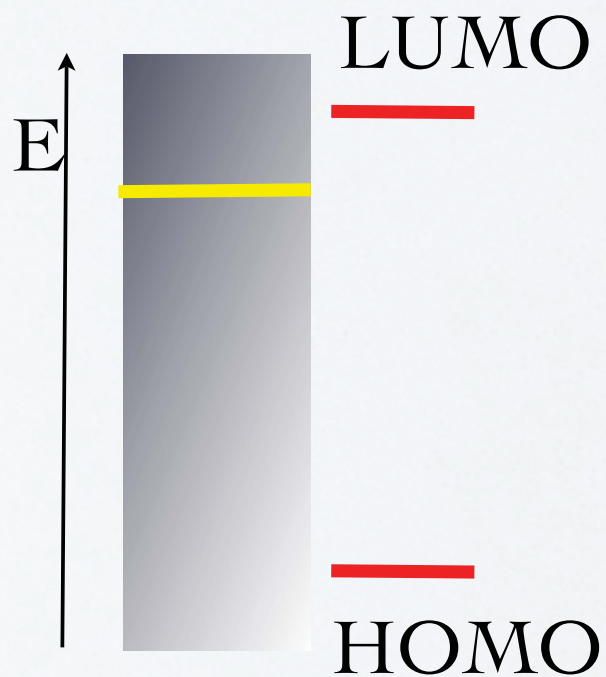
$\text{ETiO}_2/\text{DYE}^+$ injection

Charge Transfer Processes



$E_{\text{TiO}_2}/\text{DYE}^+$ injection

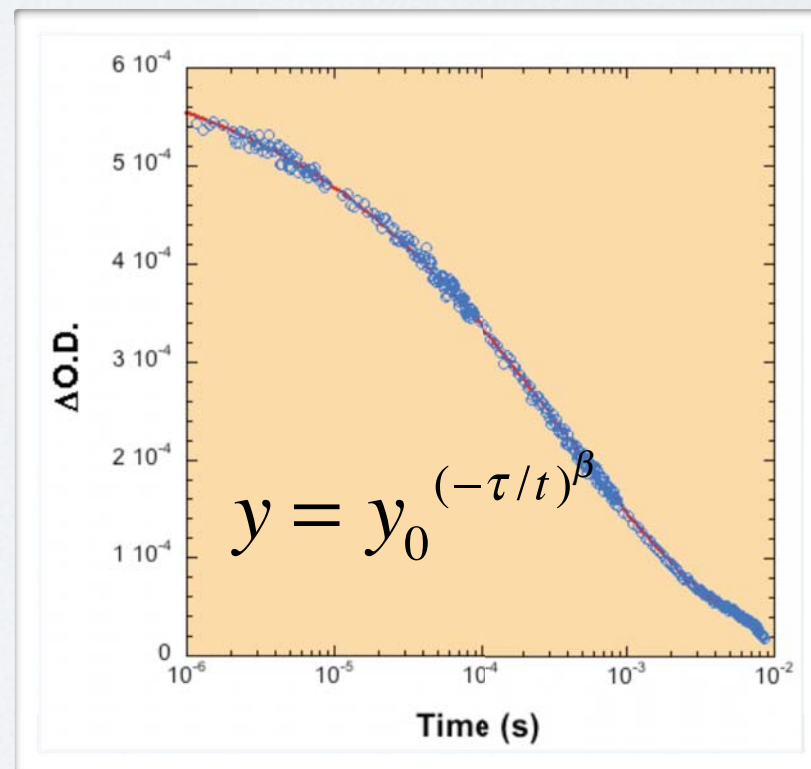
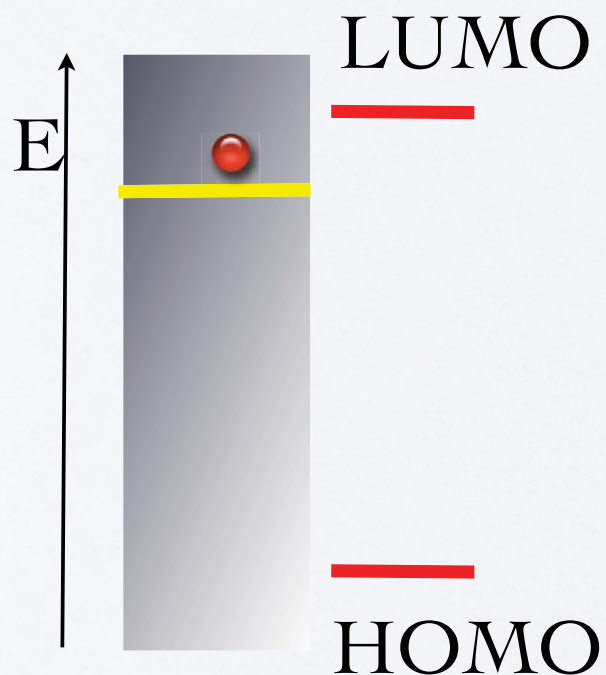
Charge Transfer Processes



Fitting to KWW function

E_{TIO_2}/DYE^+ recombination

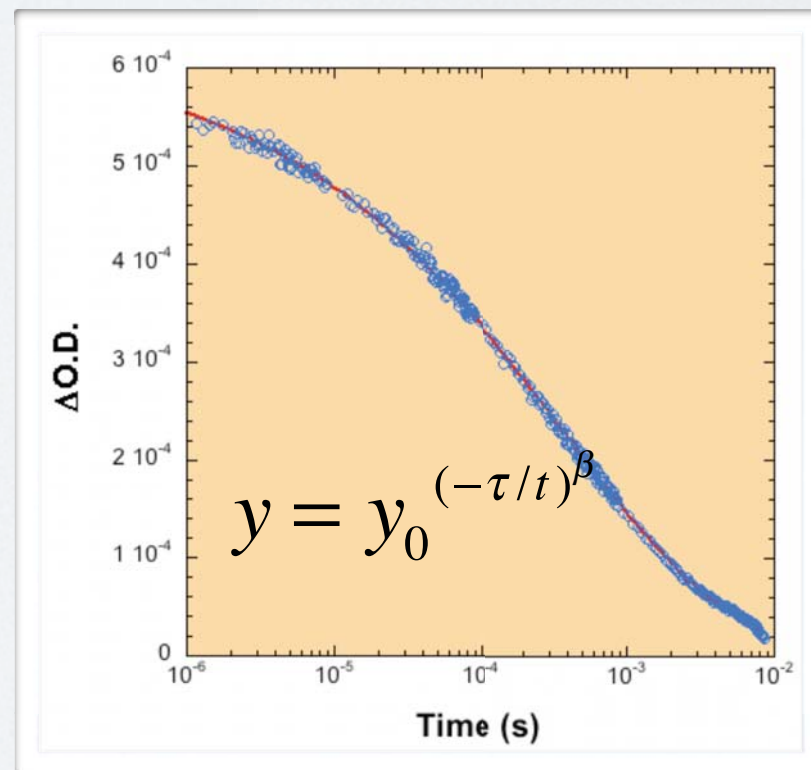
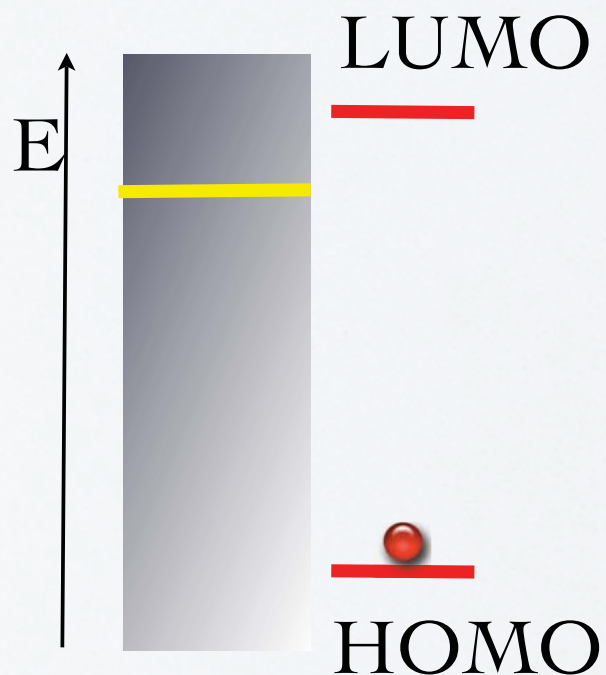
Charge Transfer Processes



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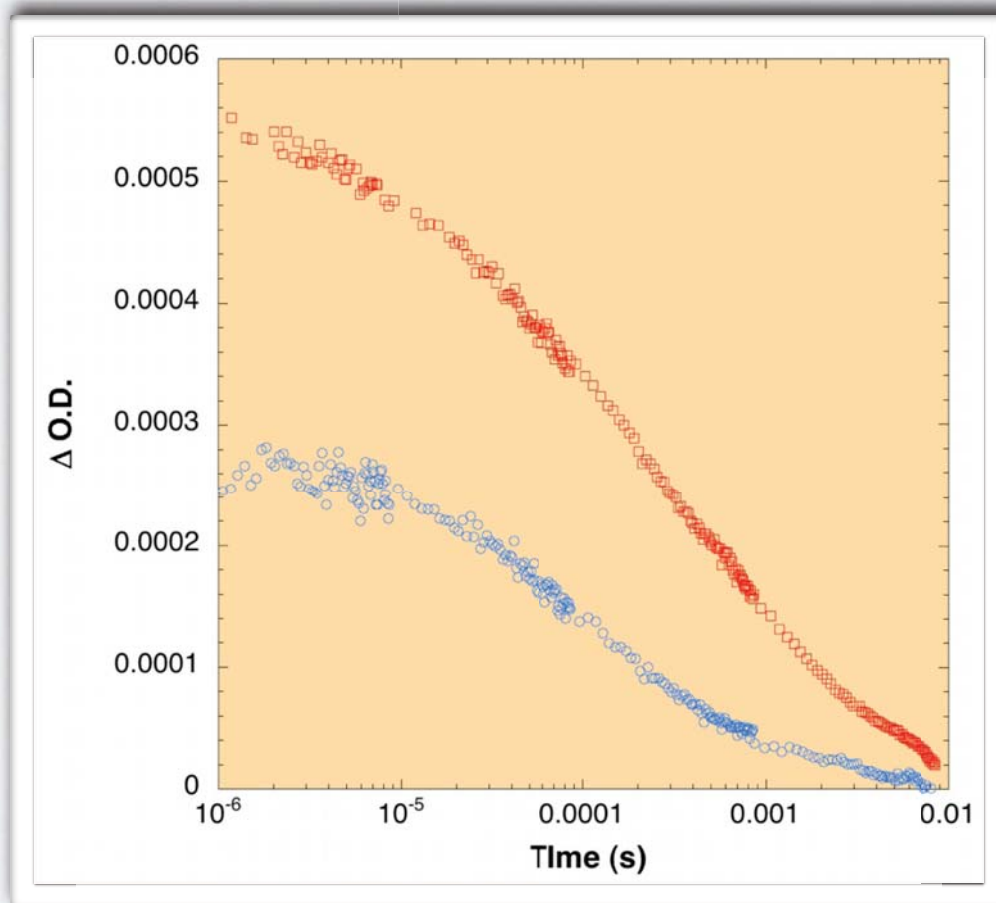
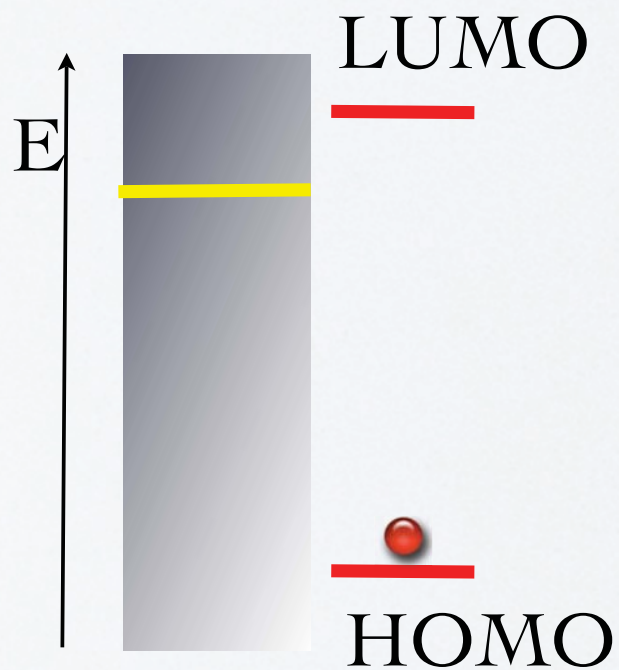
Charge Transfer Processes



Fitting to KWW function

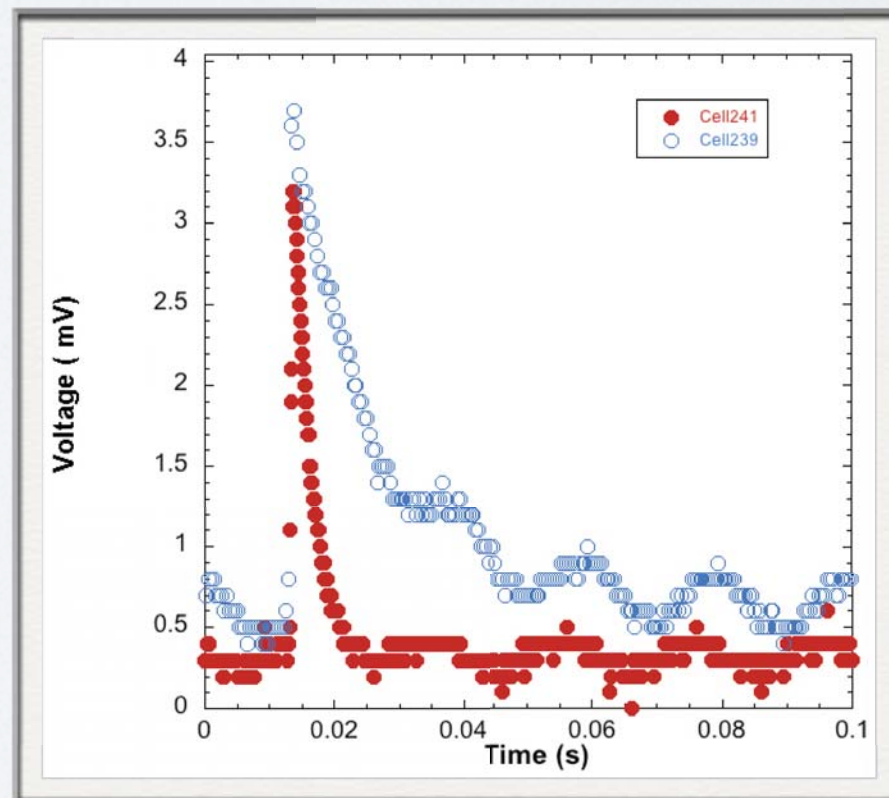
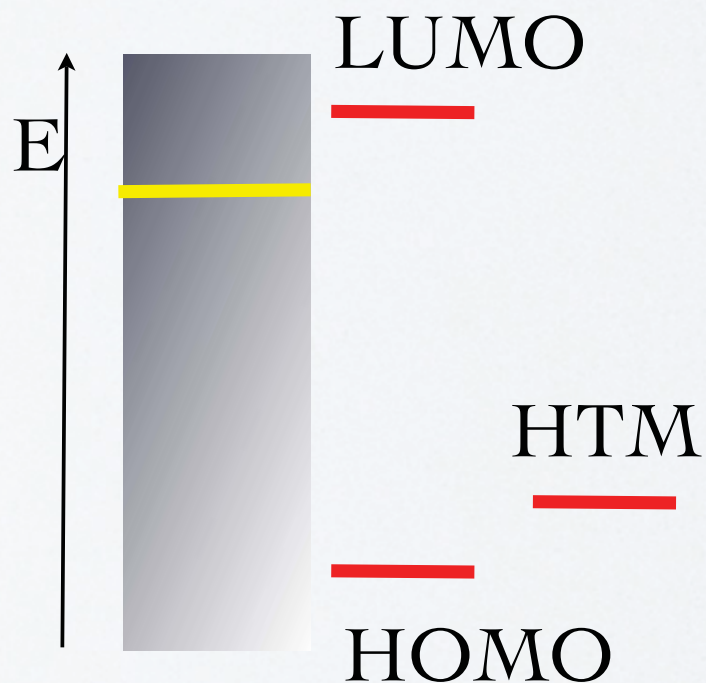
E_{TIO_2}/DYE^+ recombination

Charge Transfer Processes



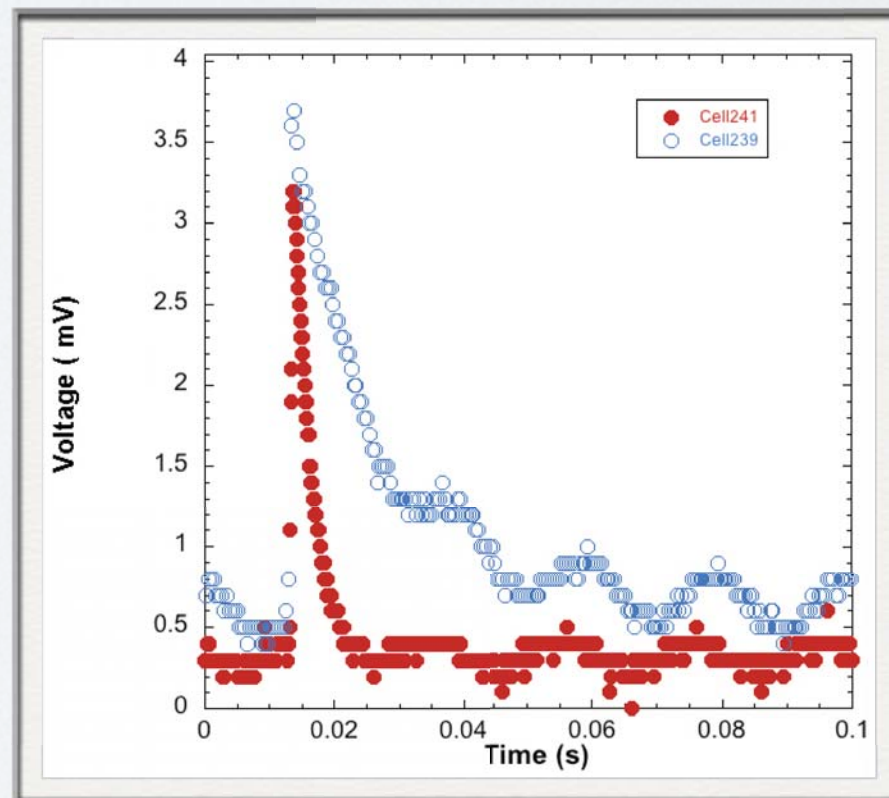
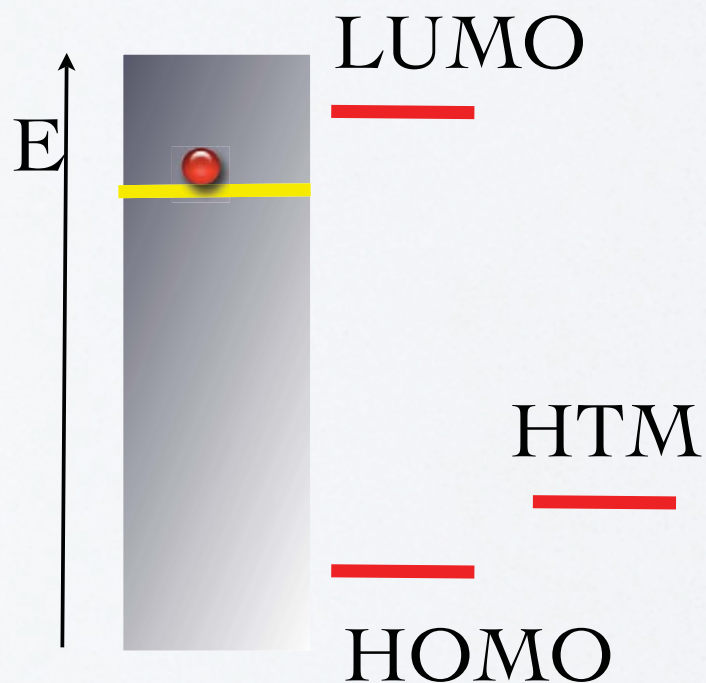
E_{TiO_2}/DYE^+ RECOMBINATION

Charge Transfer Processes



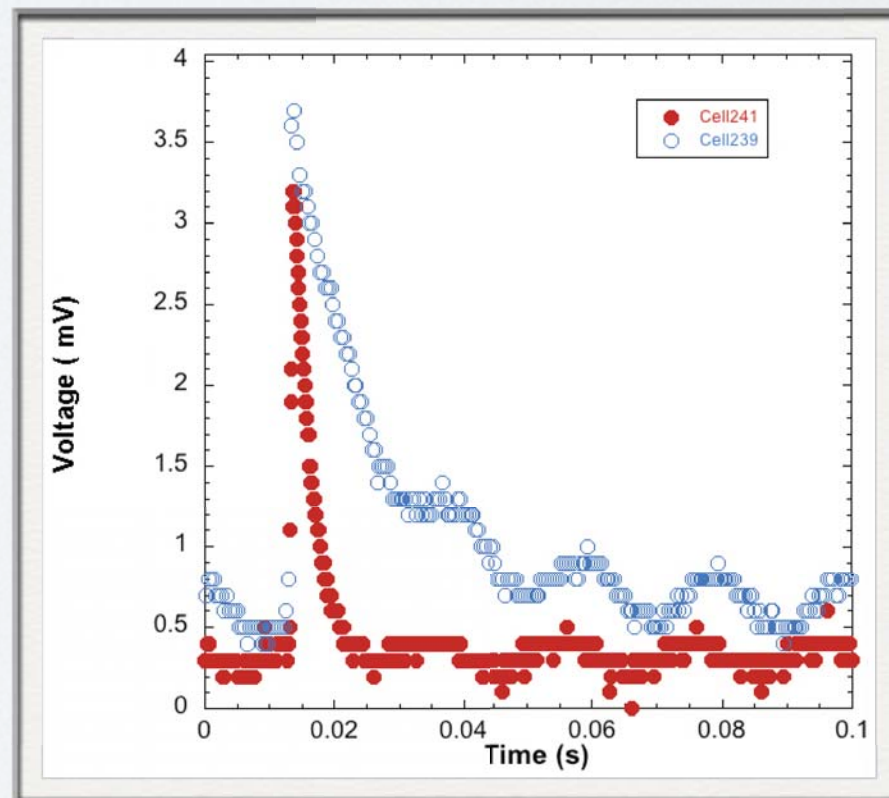
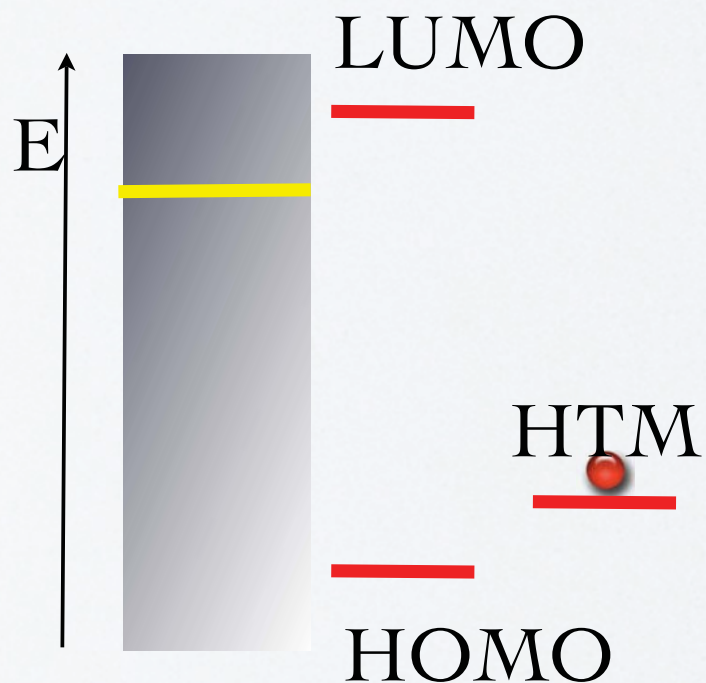
E_{TiO_2}/HTM RECOMBINATION

Charge Transfer Processes



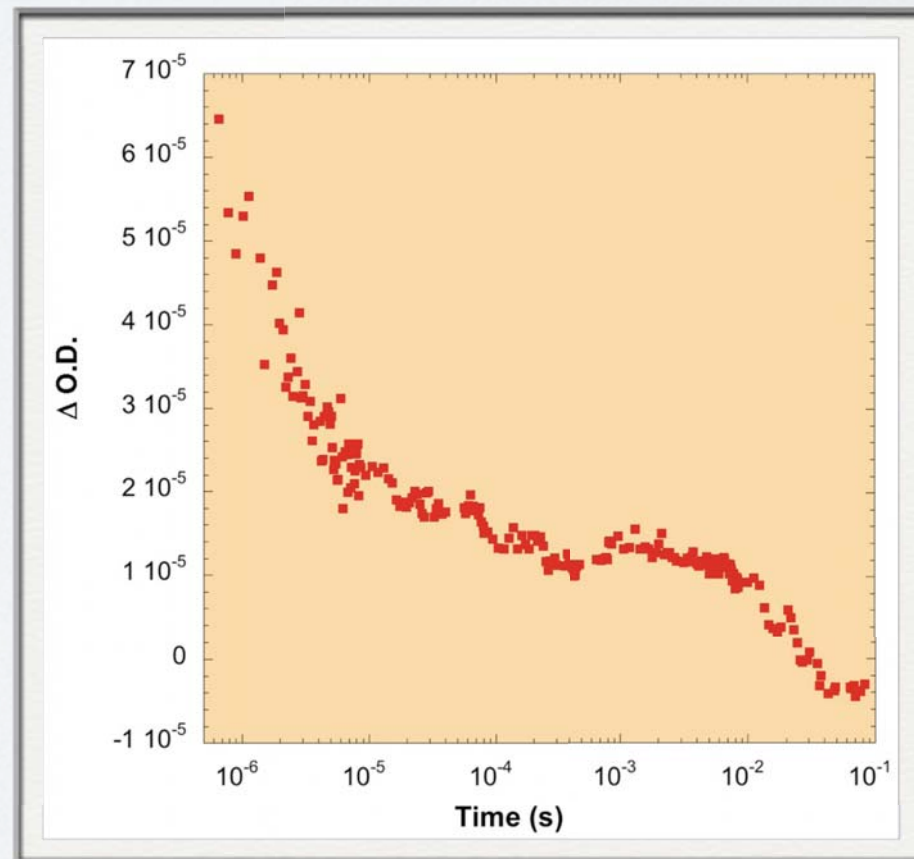
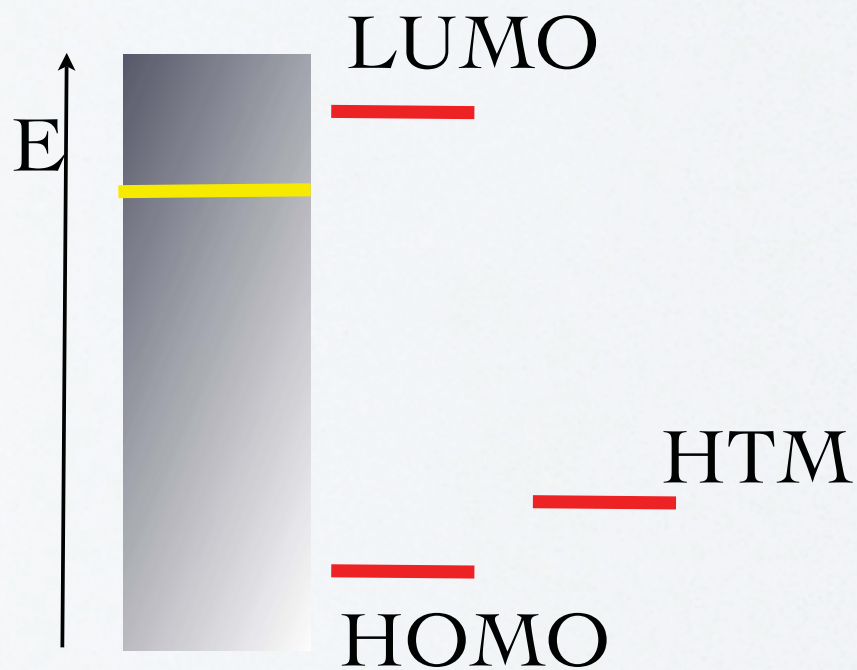
E_{TiO_2}/HTM RECOMBINATION

Charge Transfer Processes



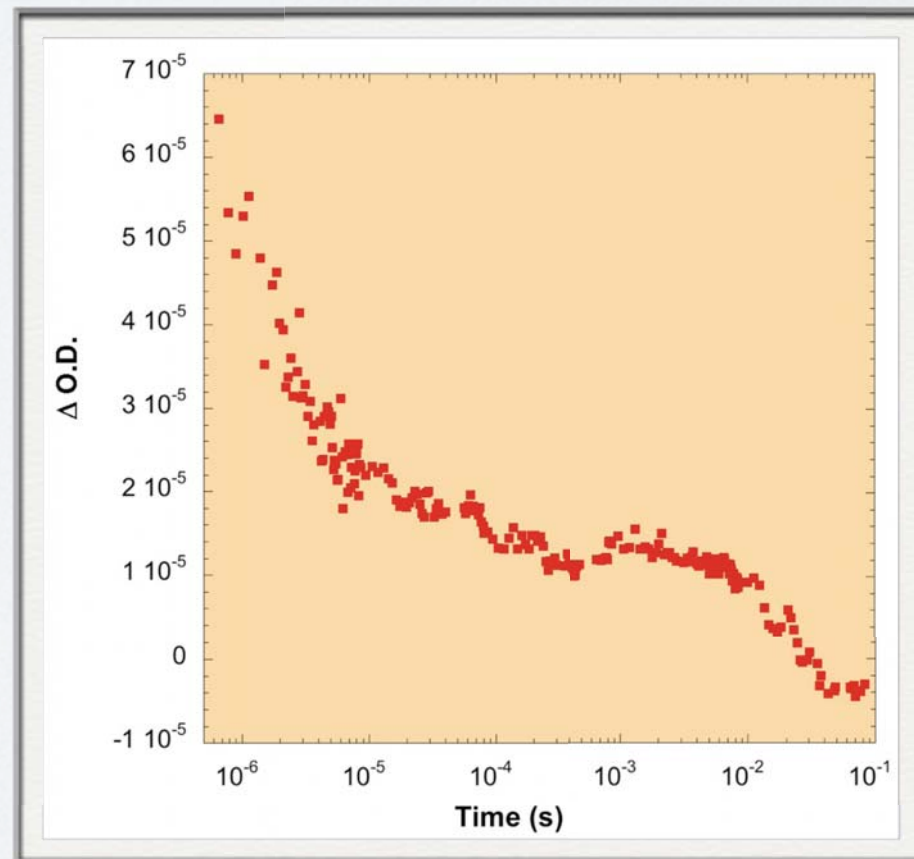
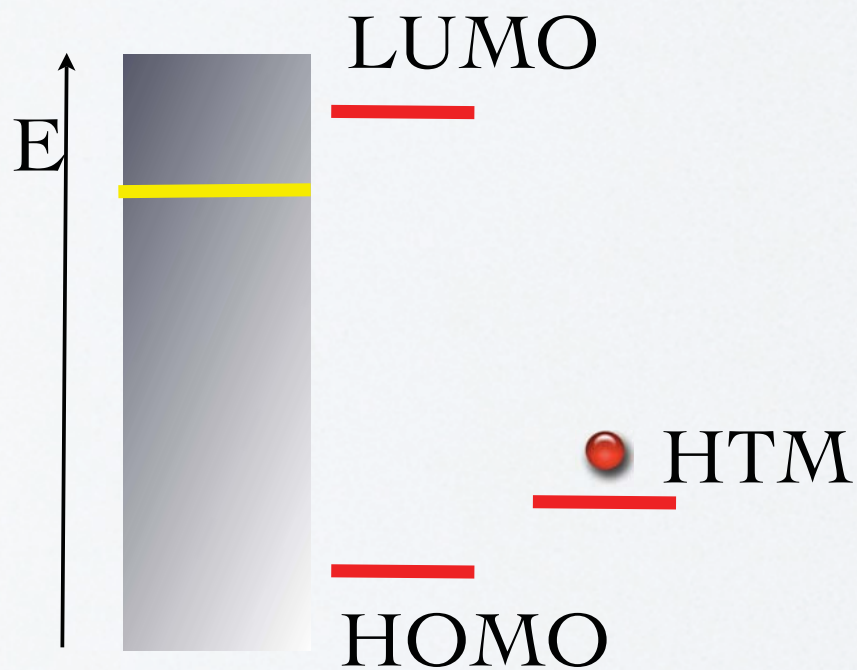
ETiO_2 /HTM RECOMBINATION

Charge Transfer Processes



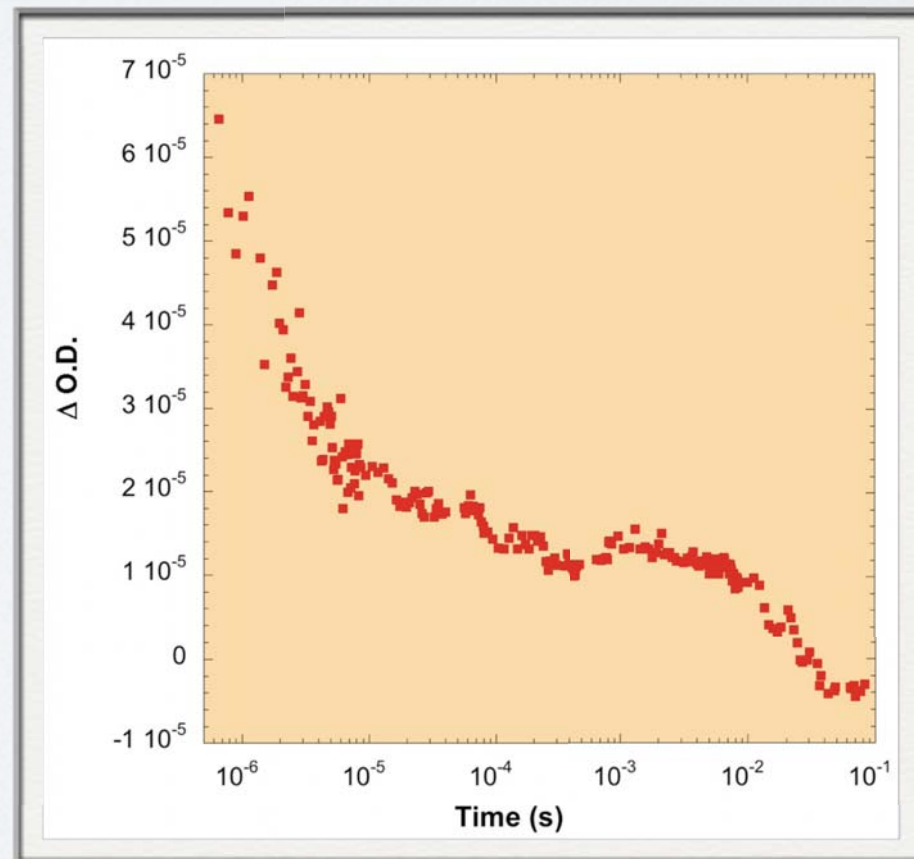
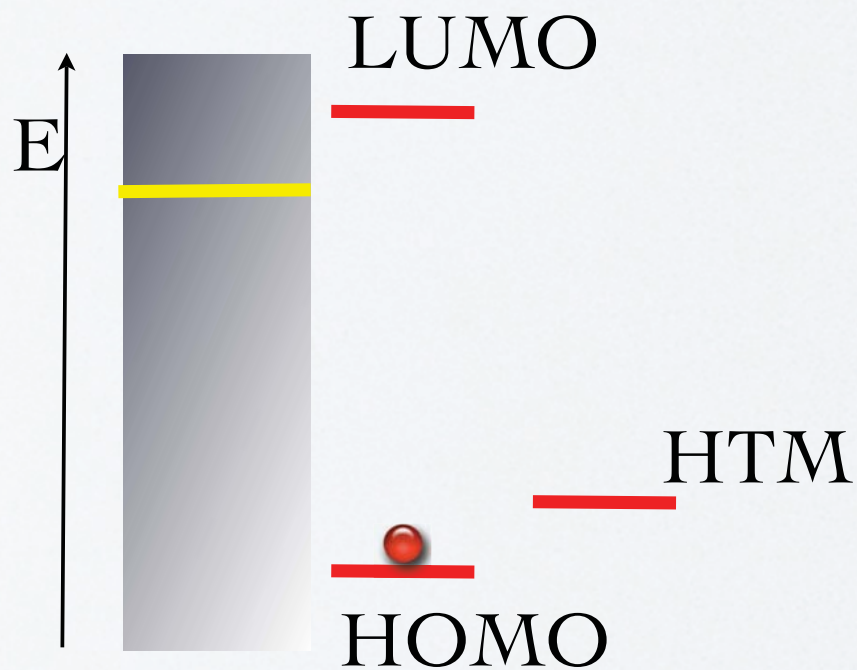
HTM/DYE⁺ Regeneration

Charge Transfer Processes



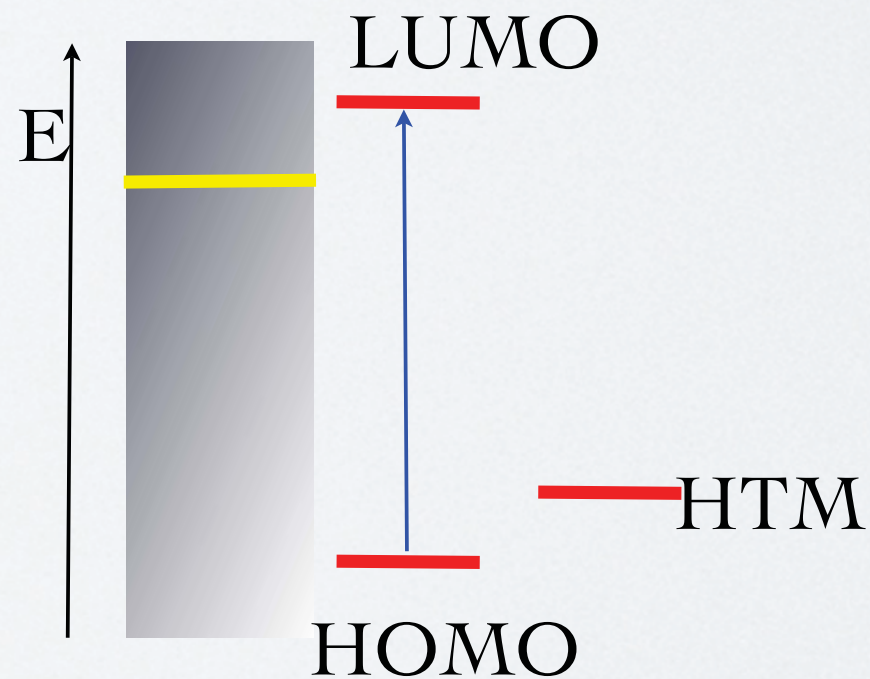
HTM/DYE⁺ Regeneration

Charge Transfer Processes



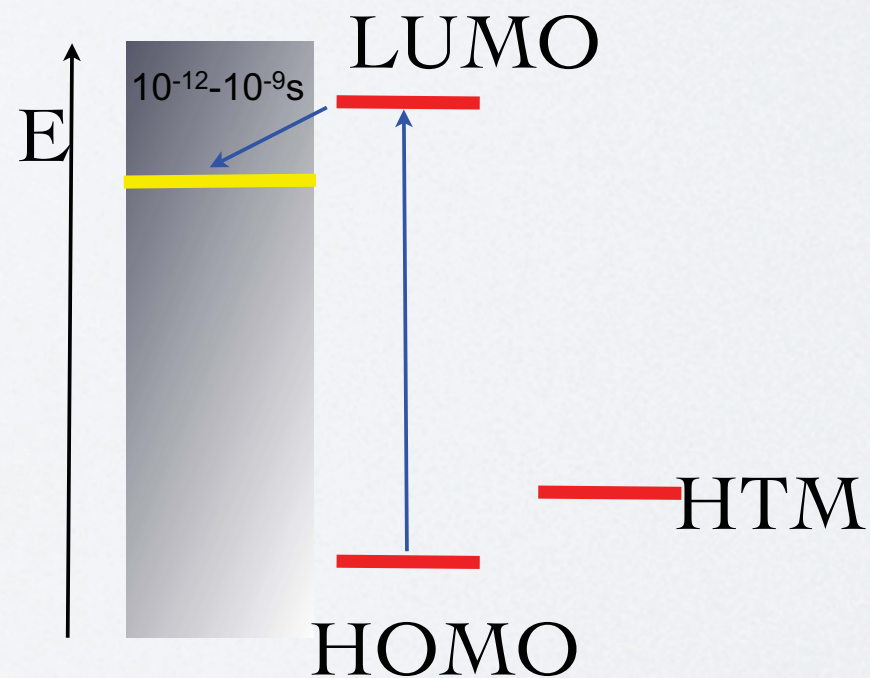
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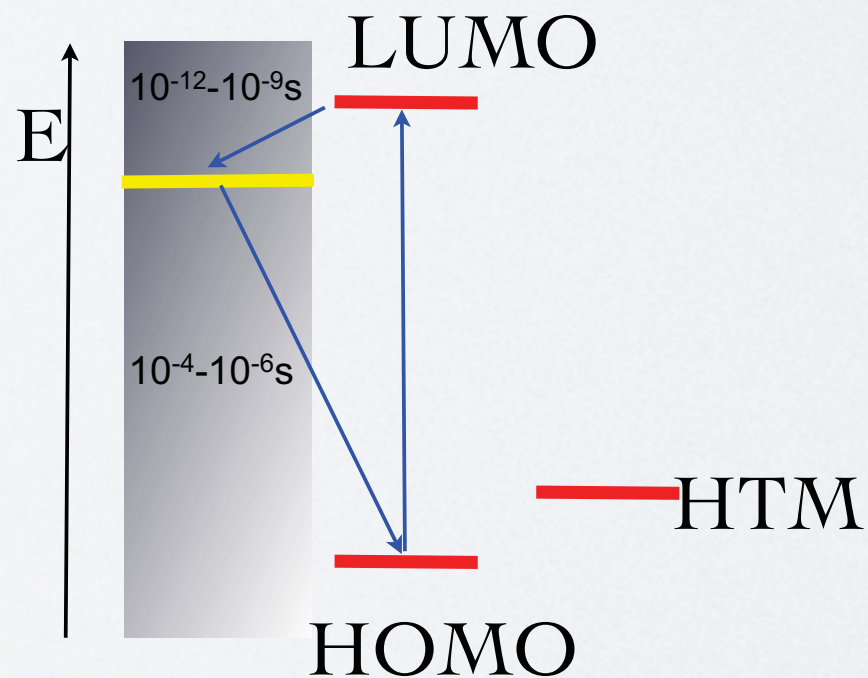
Overall charge transfer processes

Charge Transfer Processes



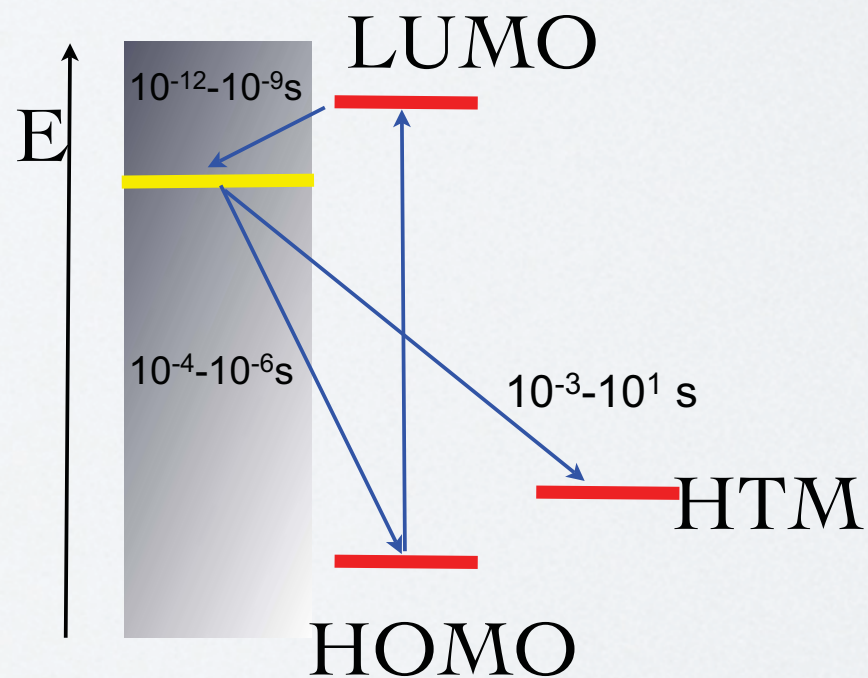
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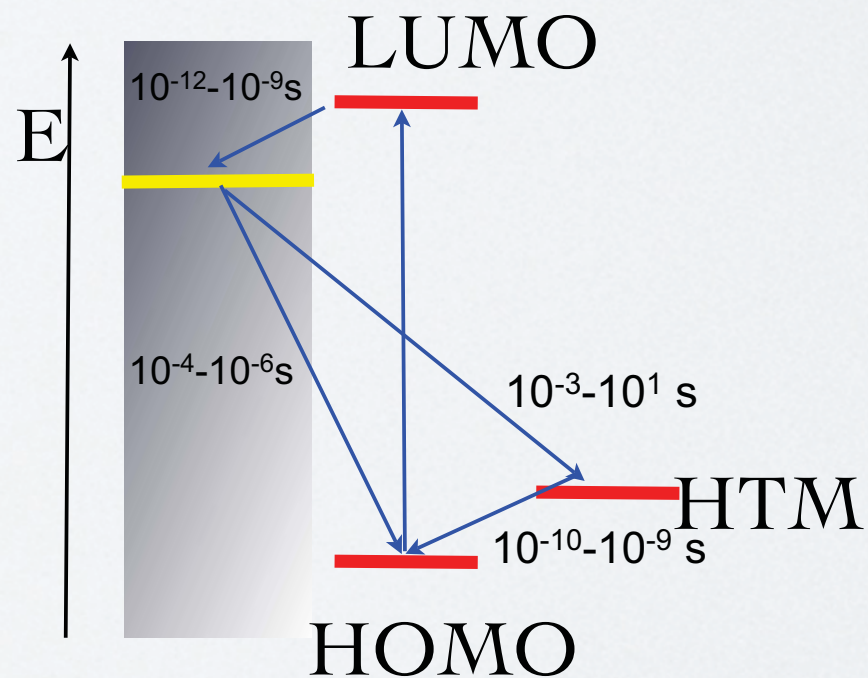
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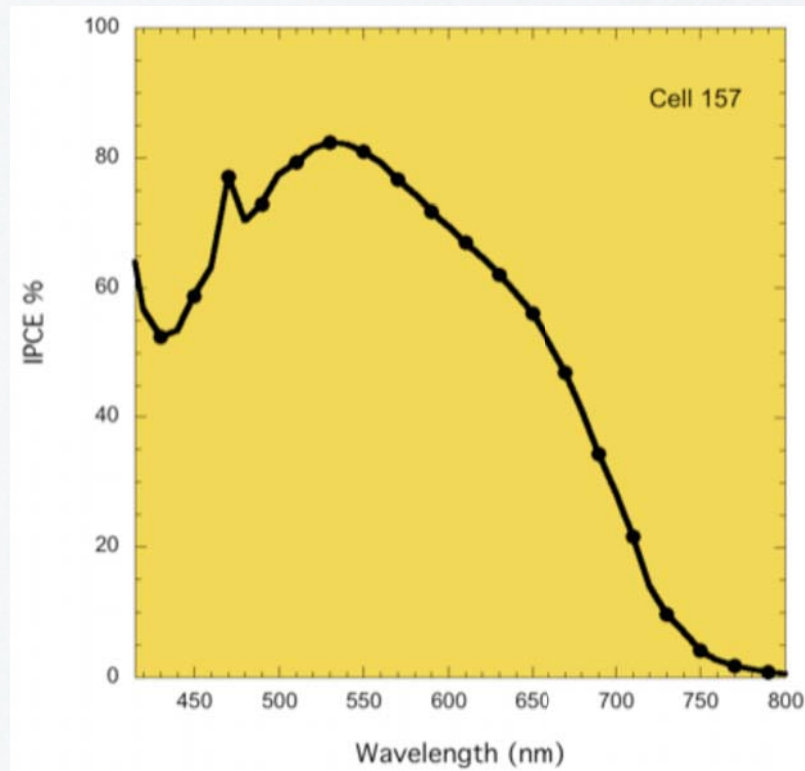
Overall charge transfer processes

Charge Transfer Processes



Overall charge transfer processes

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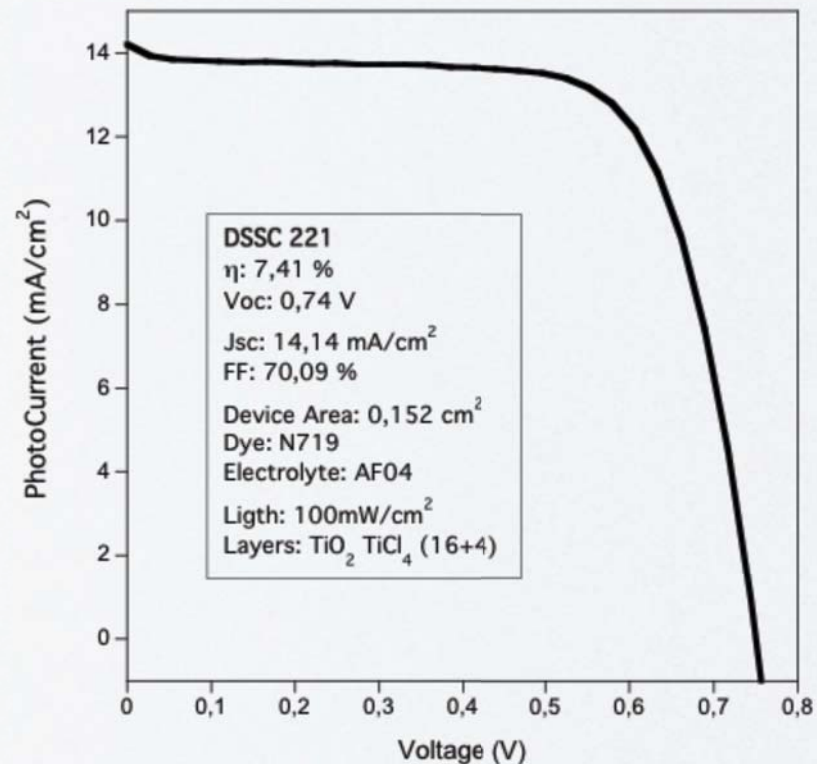


$$IPCE = \frac{I_{ph} \times 1240}{\lambda \times P_0} \times 100$$

$$\eta_{device} = I_{sc} \times V_{oc} \times FF$$

Device Characterisation

Charge Transfer Processes

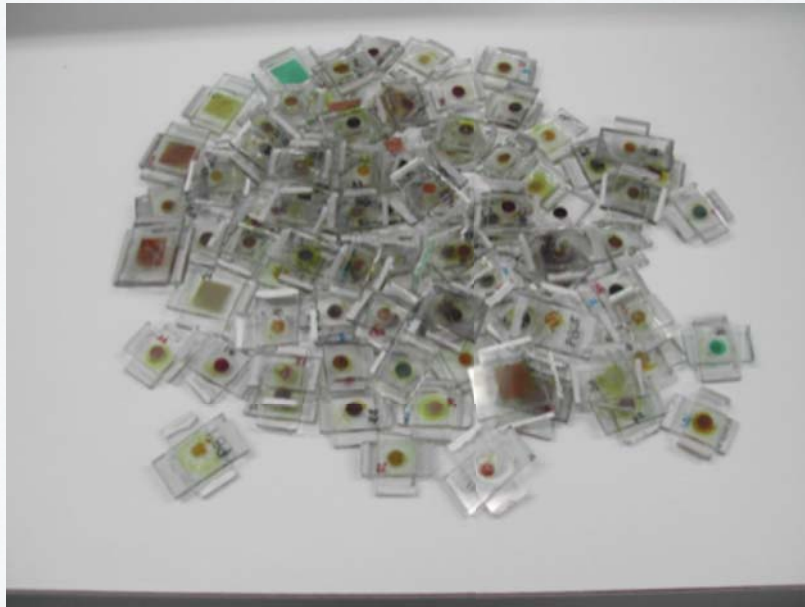


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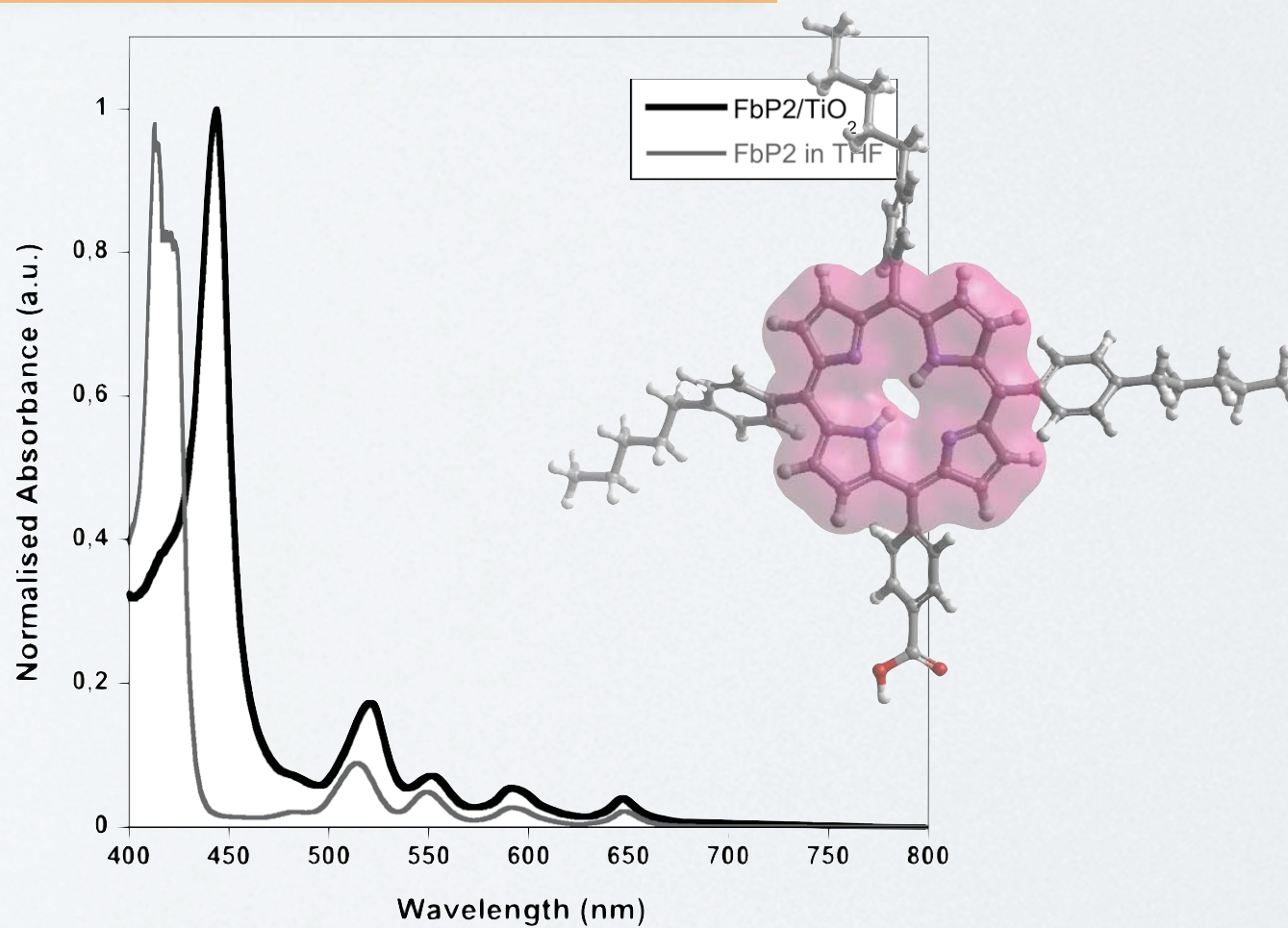


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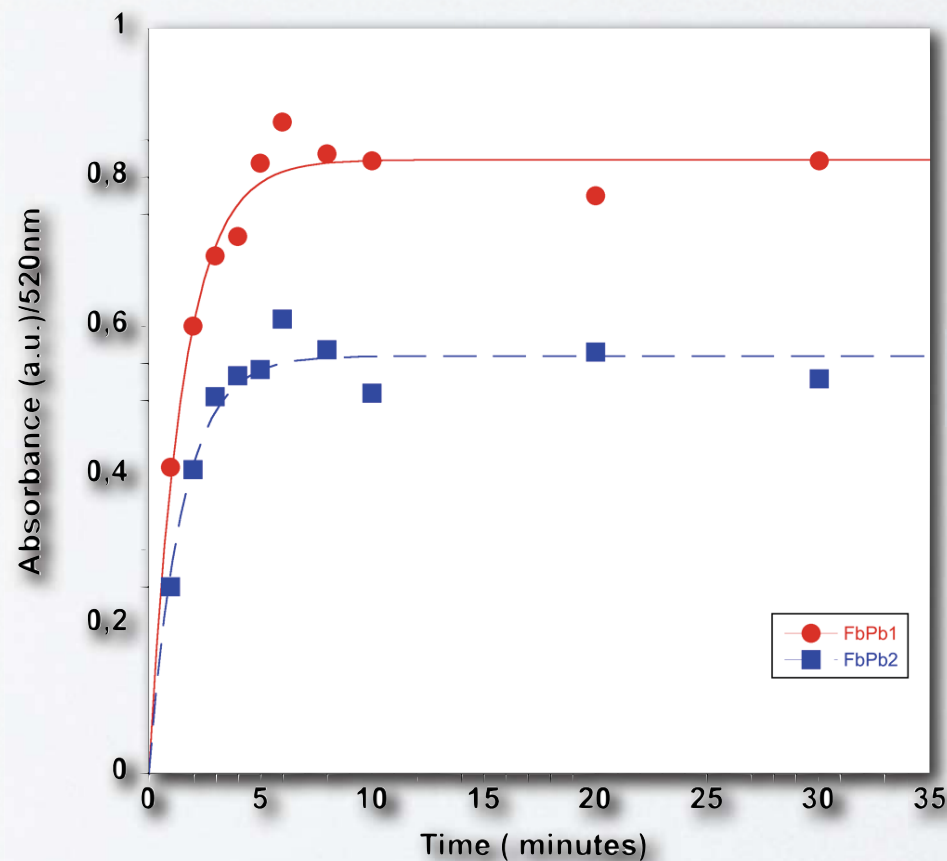
Device Characterisation

ICIQ's Research



Controlling "Dark" Electron transfer Reaction

ICIQ's Research



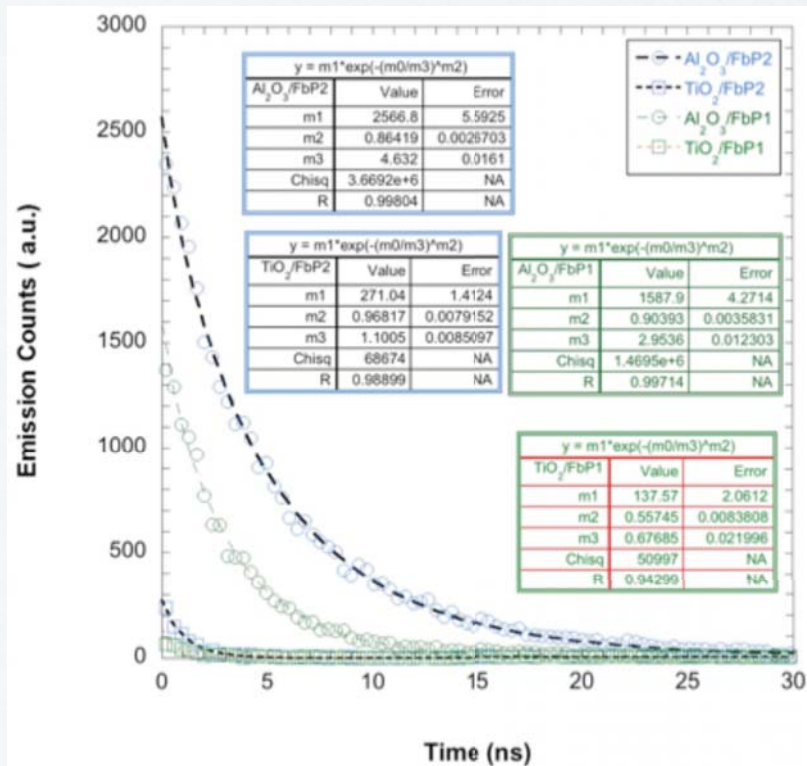
Dye absorption Kinetics

$$A = A_{\max} (1 - \exp(-K_{ads}t))$$

● Lagergren's Equation

Controlling "Dark" Electron transfer Reaction

ICIQ's Research



Dye Injection kinetics

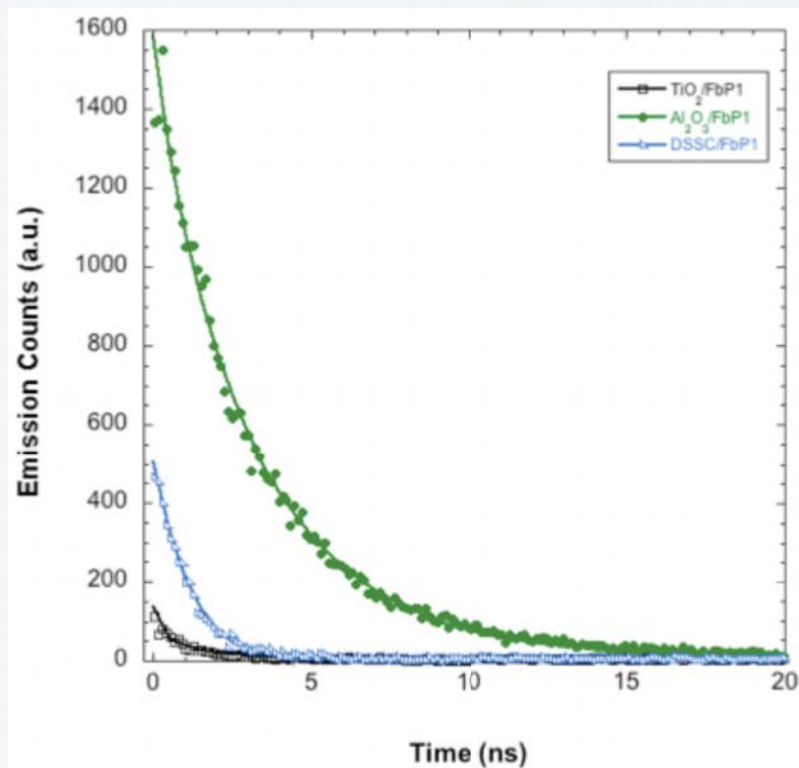
$$y = y_0 (-\tau/t)^\beta$$

Injection into TiO_2 CB occurs before 100 ps

Injection on Devices is slower.
Nonetheless still faster than 250 ps

Controlling "Dark" Electron transfer Reaction

ICIQ's Research



Dye Injection kinetics

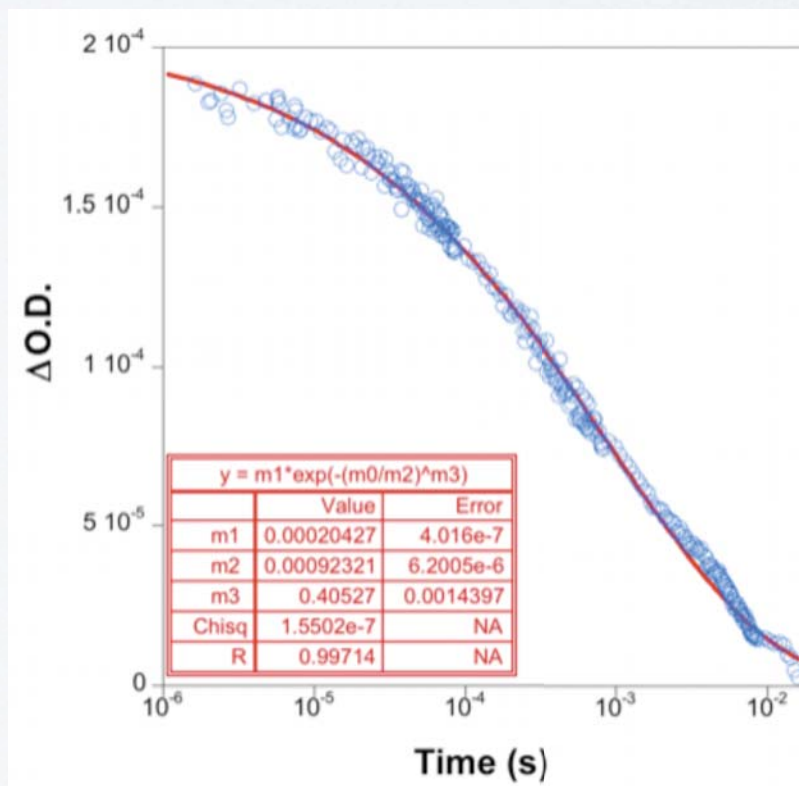
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Controlling "Dark" Electron transfer Reaction

ICIQ's Research



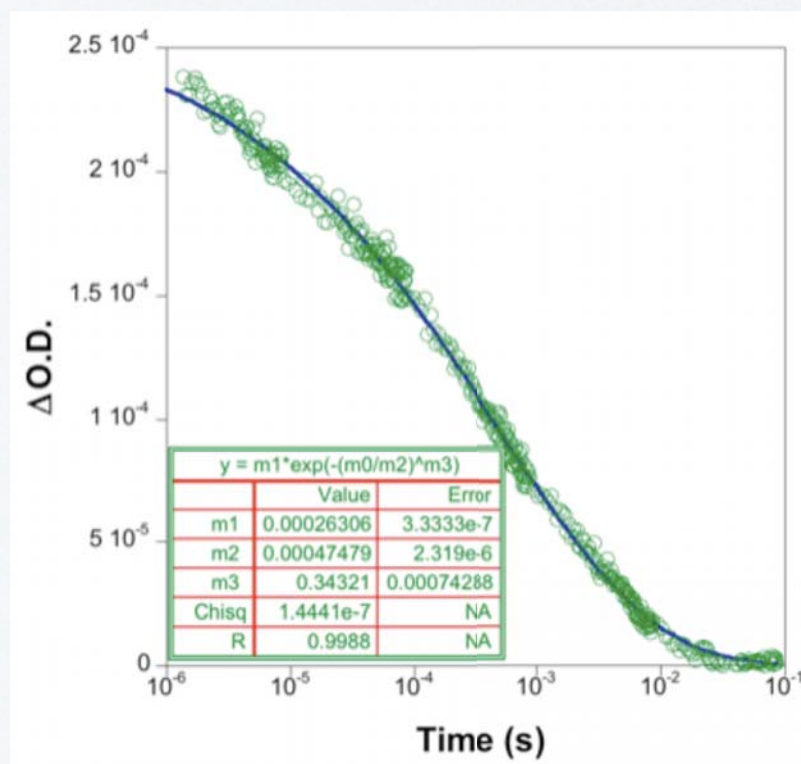
TiO₂/Dye⁺ charge transfer kinetics

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● TiO₂/dye⁺ recombination half-lifetime $\sim 3 \times 10^{-4}$ s.

Controlling "Dark" Electron transfer Reaction

ICIQ's Research



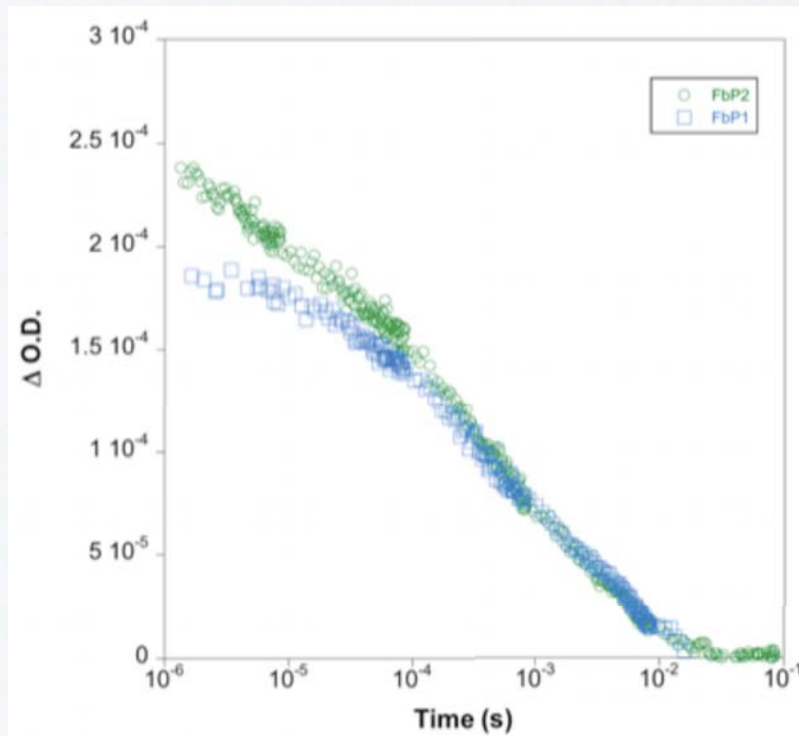
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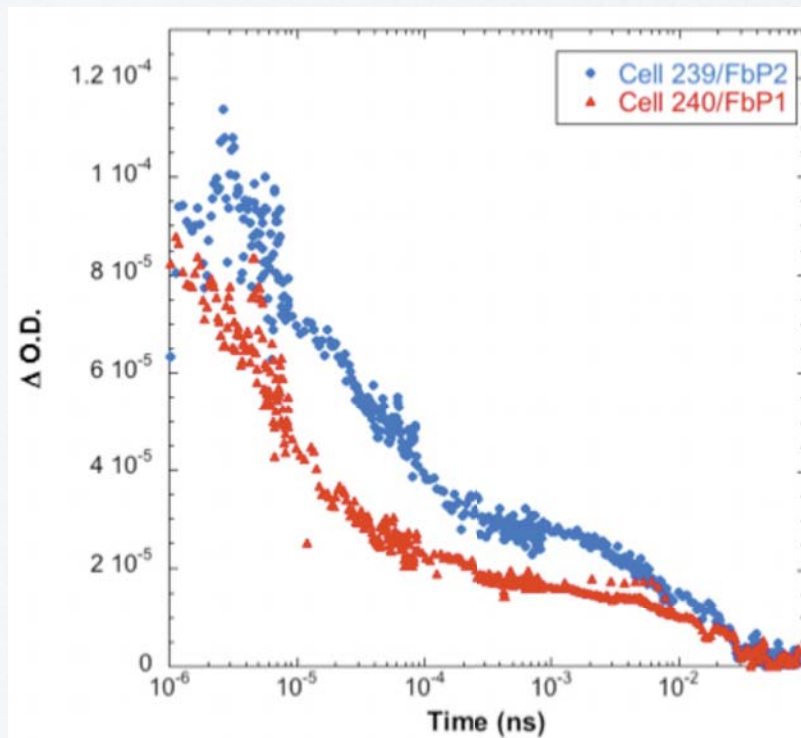
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Controlling "Dark" Electron transfer Reaction

ICIQ's Research



TiO₂/Dye⁺ charge transfer kinetics

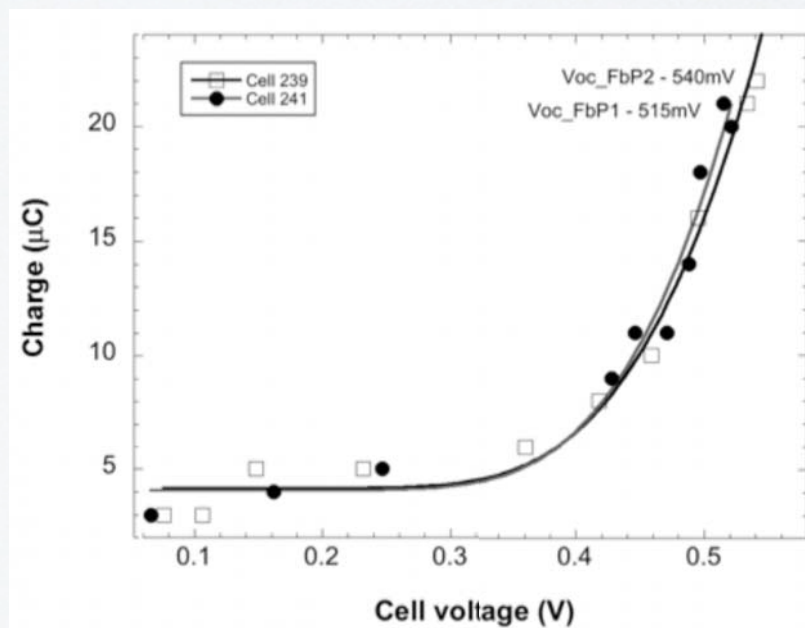
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Controlling "Dark" Electron transfer Reaction

ICIQ's Research

TiO₂/electrolyte⁺ charge transfer kinetics

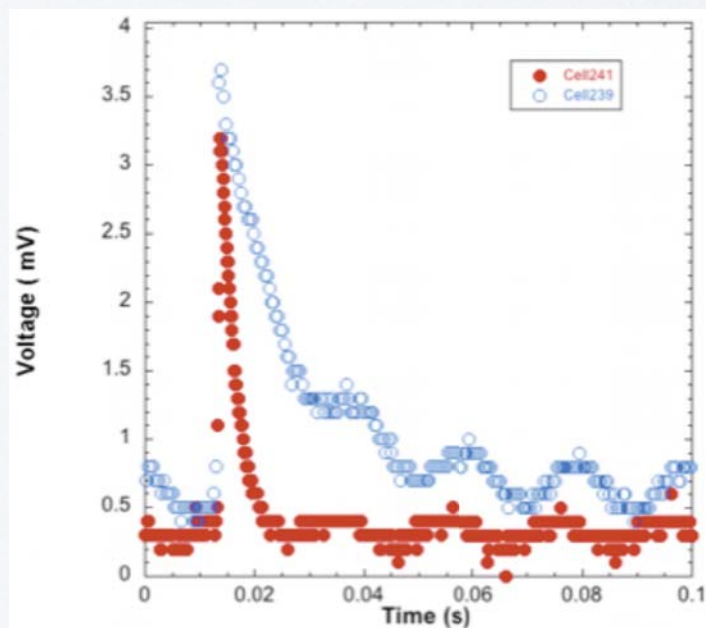


- No TiO₂ CB shift. No effect on the DOS by alkyl chains
- Slow "dark" recombination dynamics

Controlling "Dark" Electron transfer Reaction

ICIQ's Research

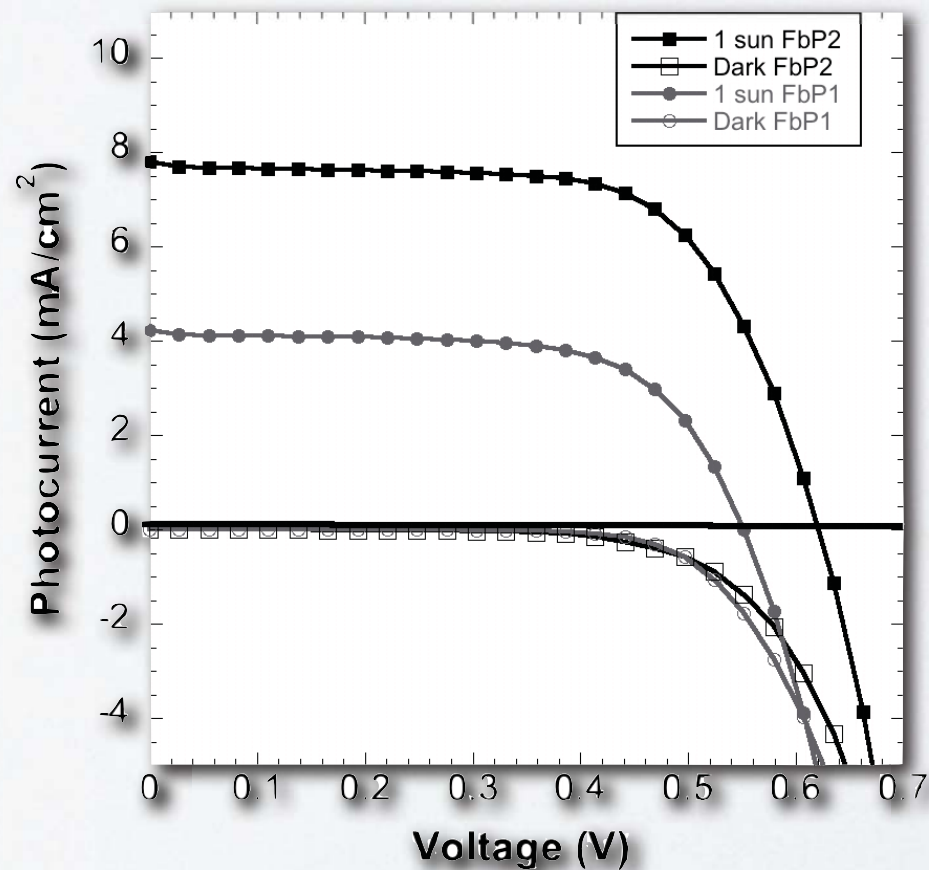
TiO₂/electrolyte⁺ charge transfer kinetics



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Controlling "Dark" Electron transfer Reaction

ICIQ's Research



DSSC Devices

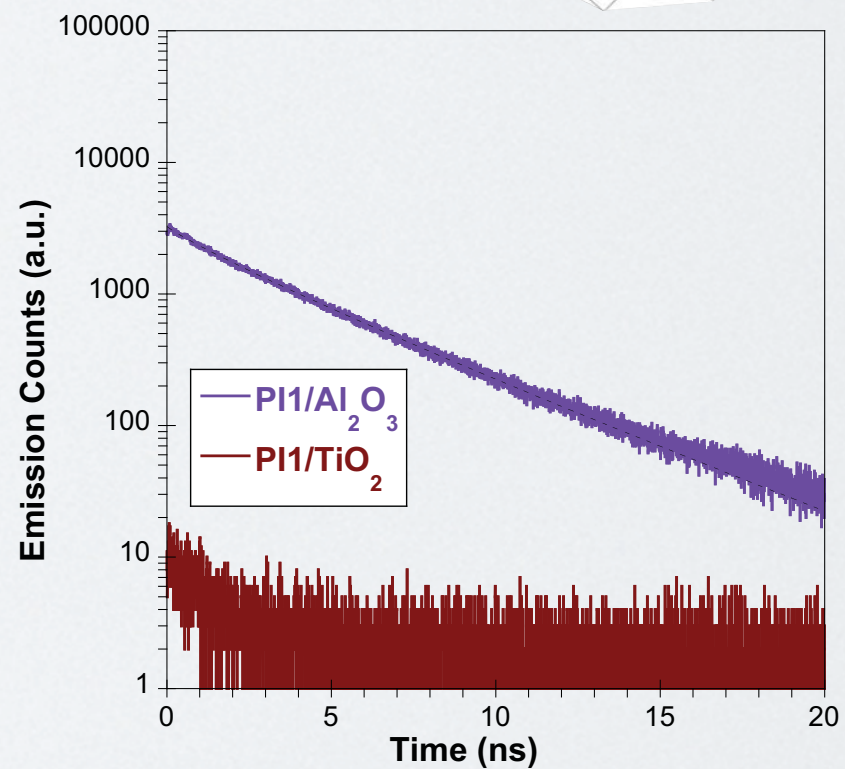
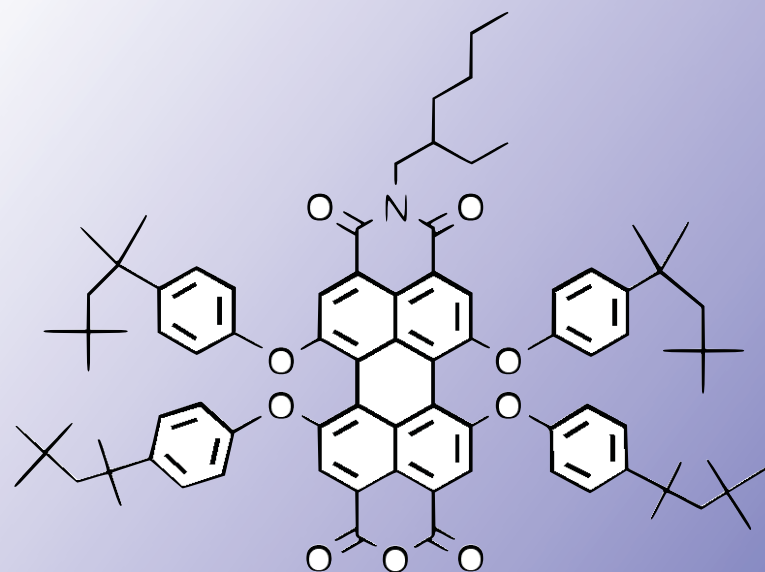
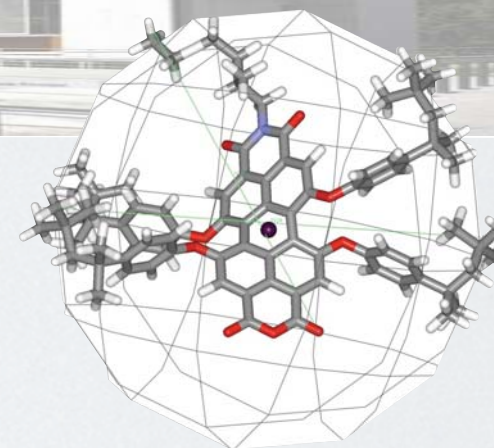
● Increase in Current

● Increase in voltage

Enhanced device efficiency

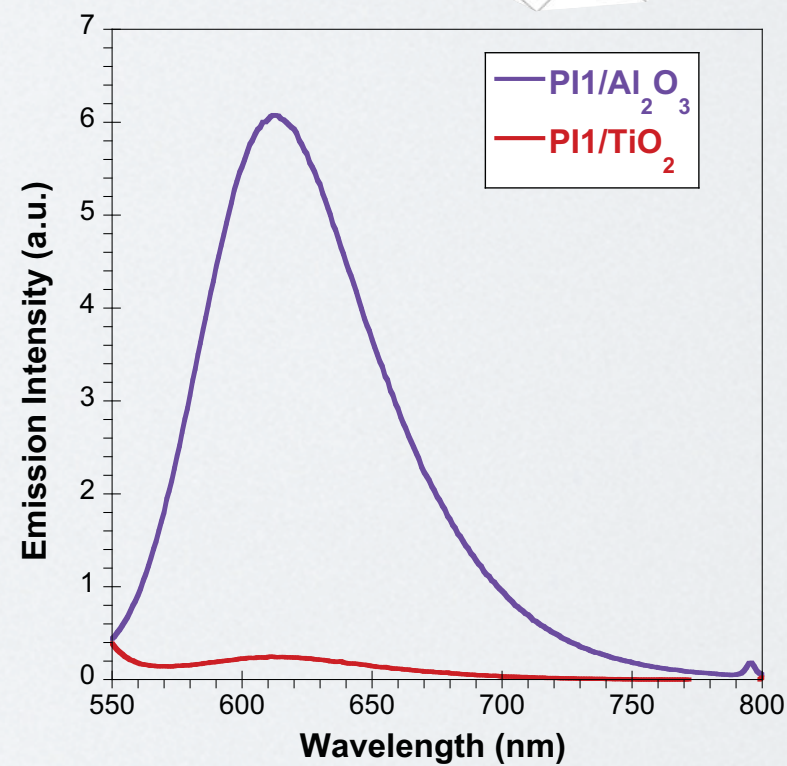
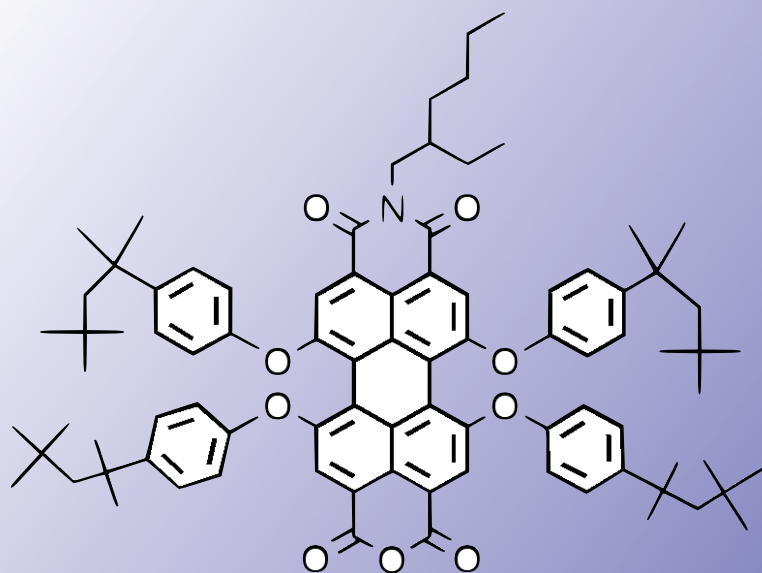
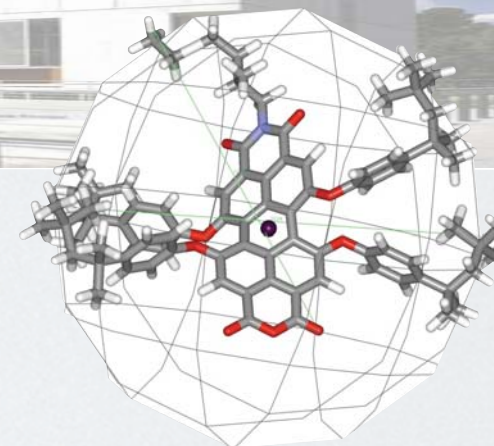


Dye Sensitised Solar Cells





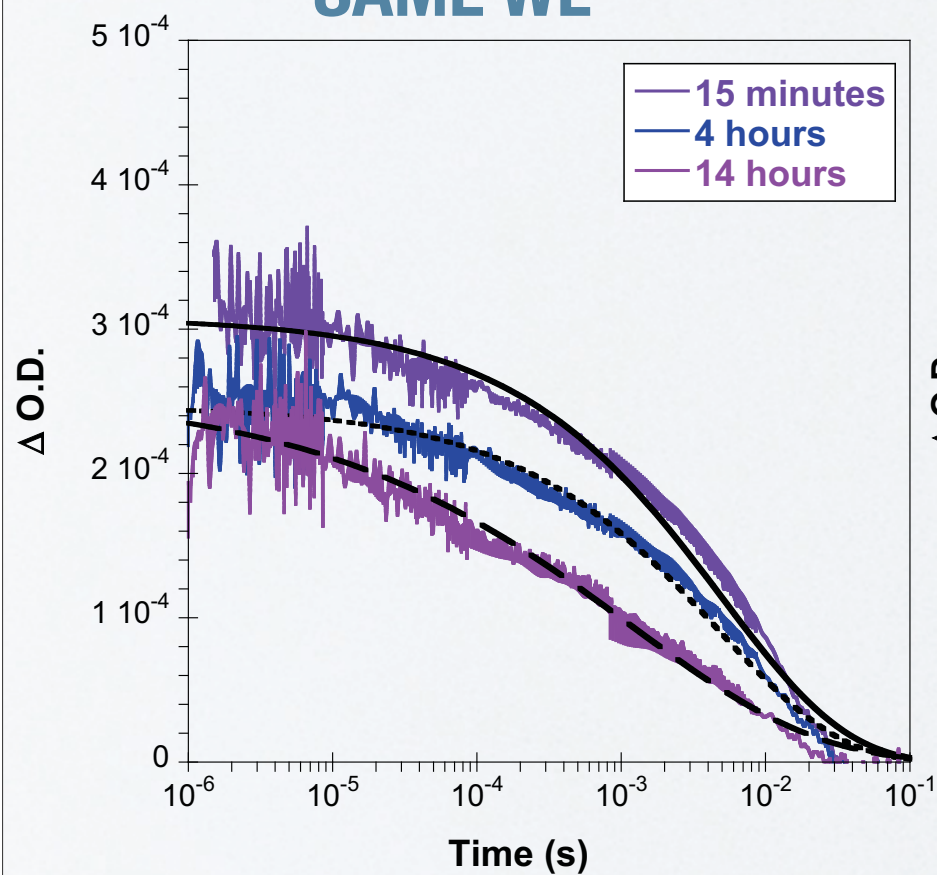
Dye Sensitised Solar Cells



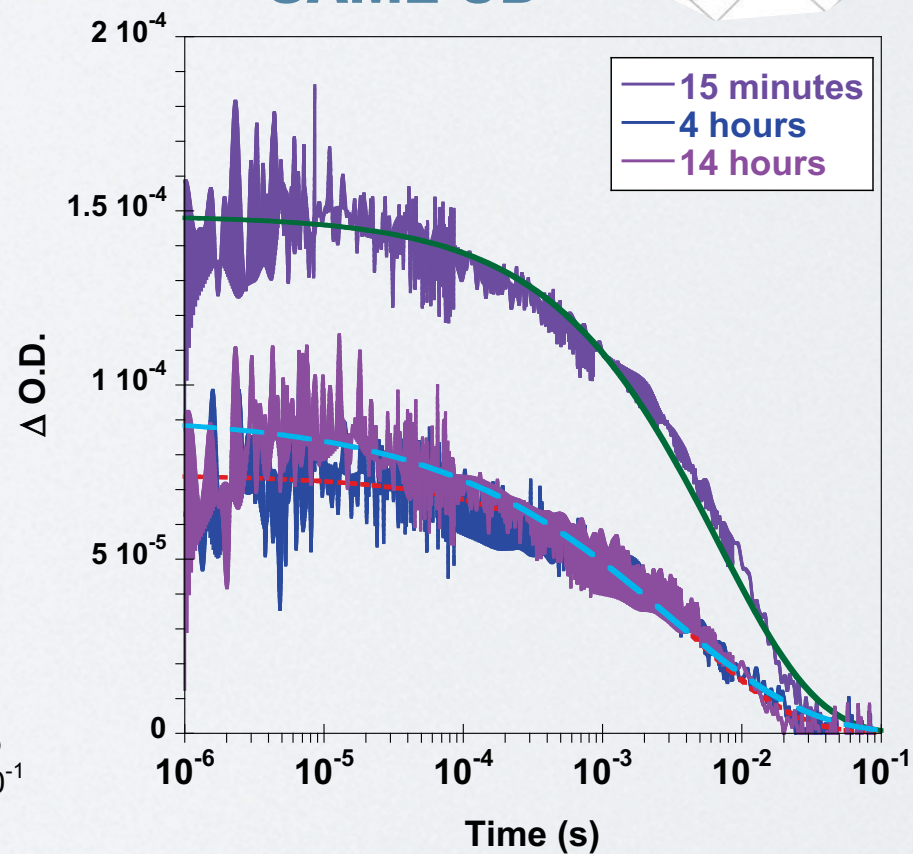


Dye Sensitised Solar Cells

SAME WL

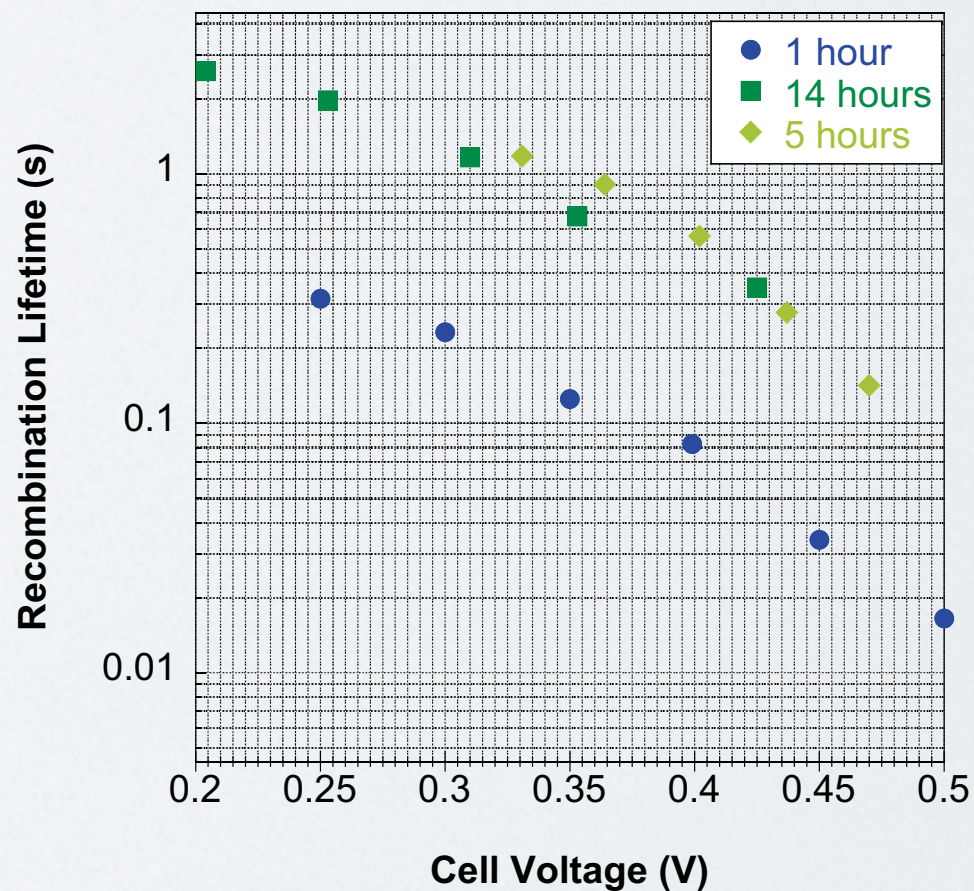
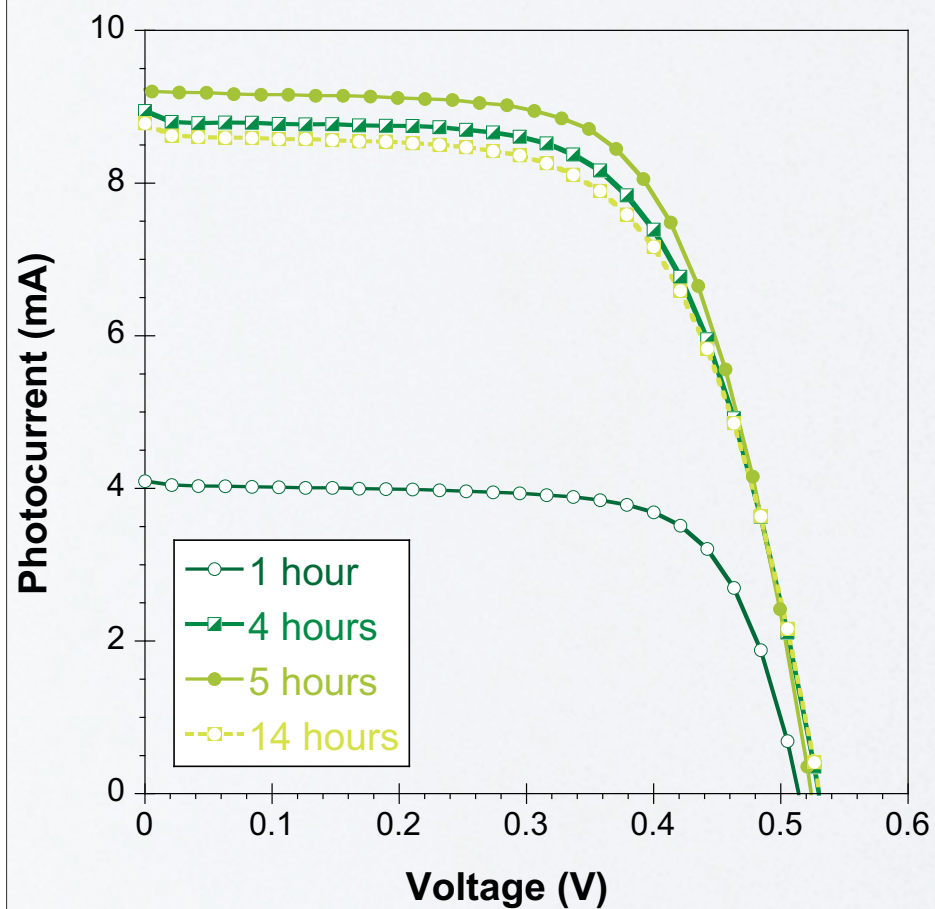
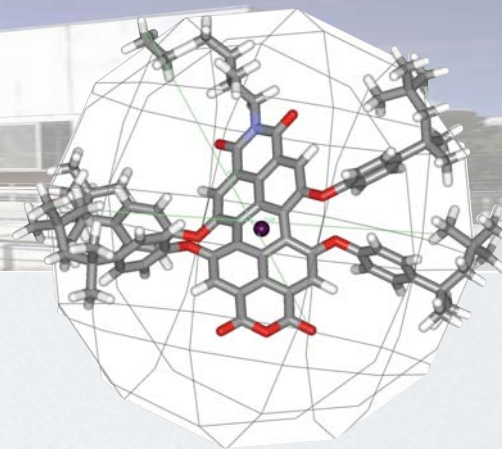


SAME OD



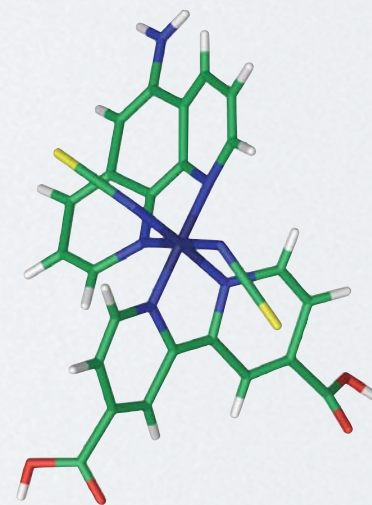
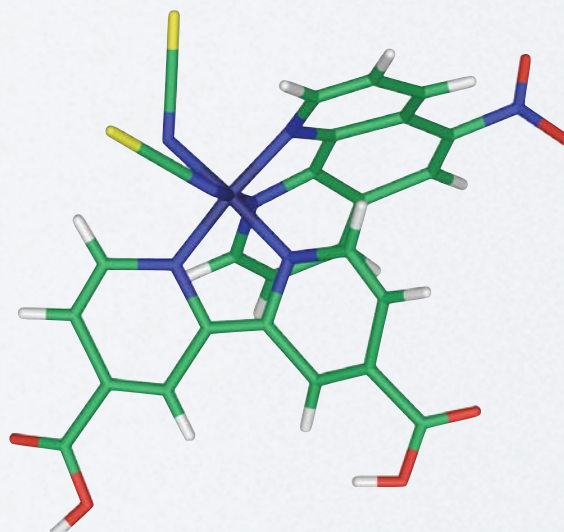
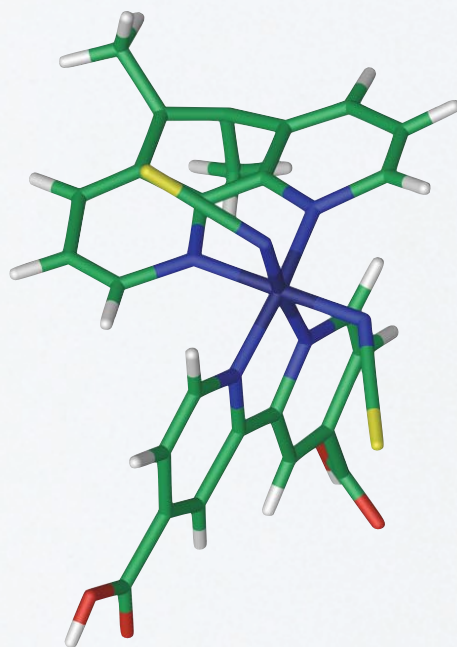


Dye Sensitised Solar Cells



Dye Sensitised Solar Cells

 ICIQ-Dyes

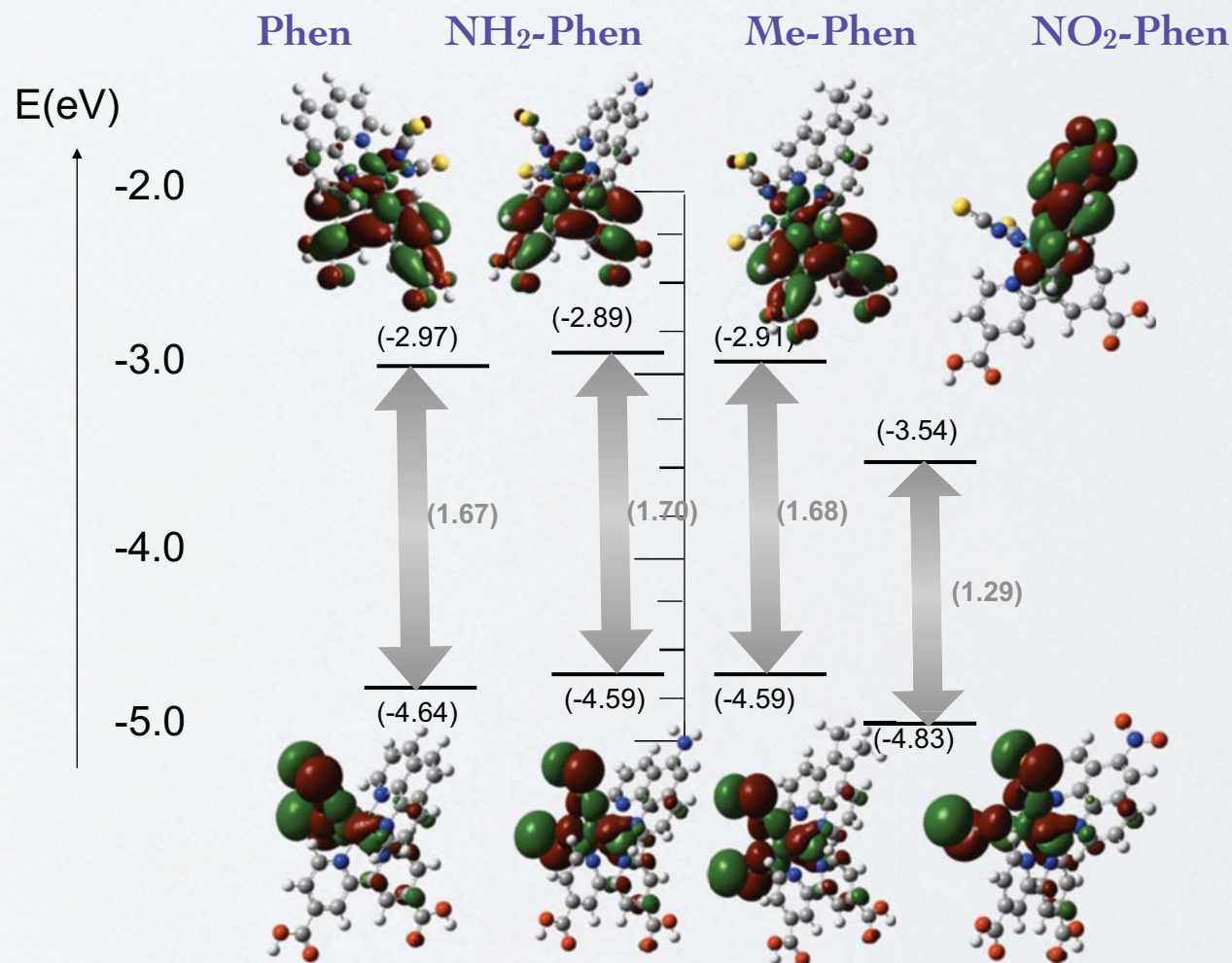


phenanthroline heteroleptic Ru(II) complexes

Dye Sensitised Solar Cells

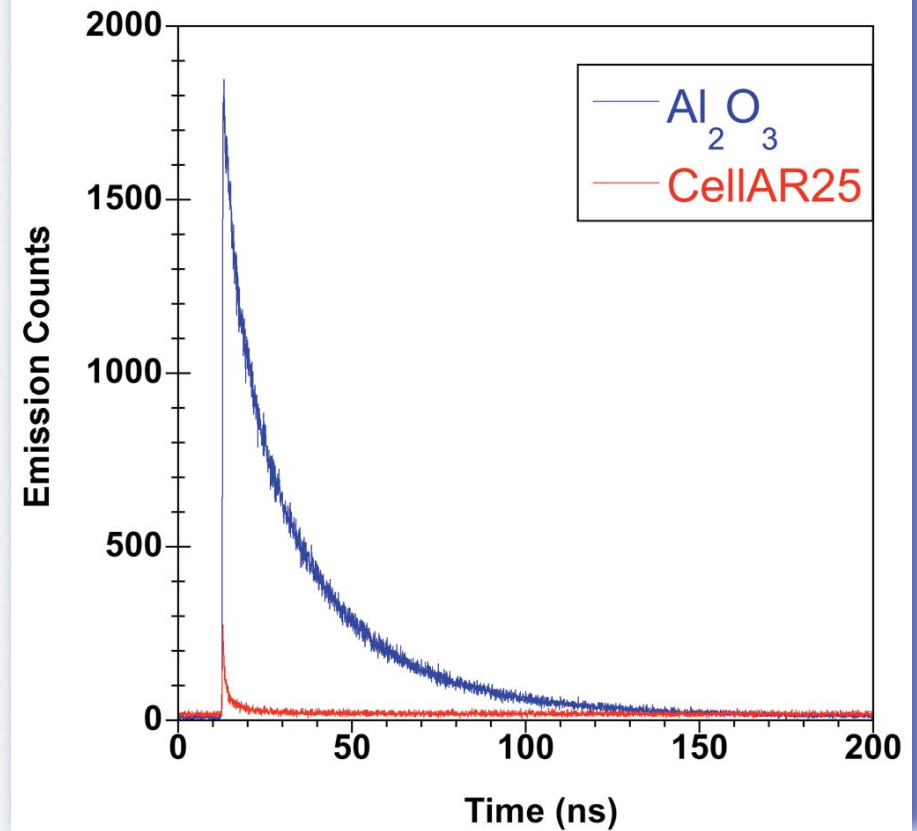
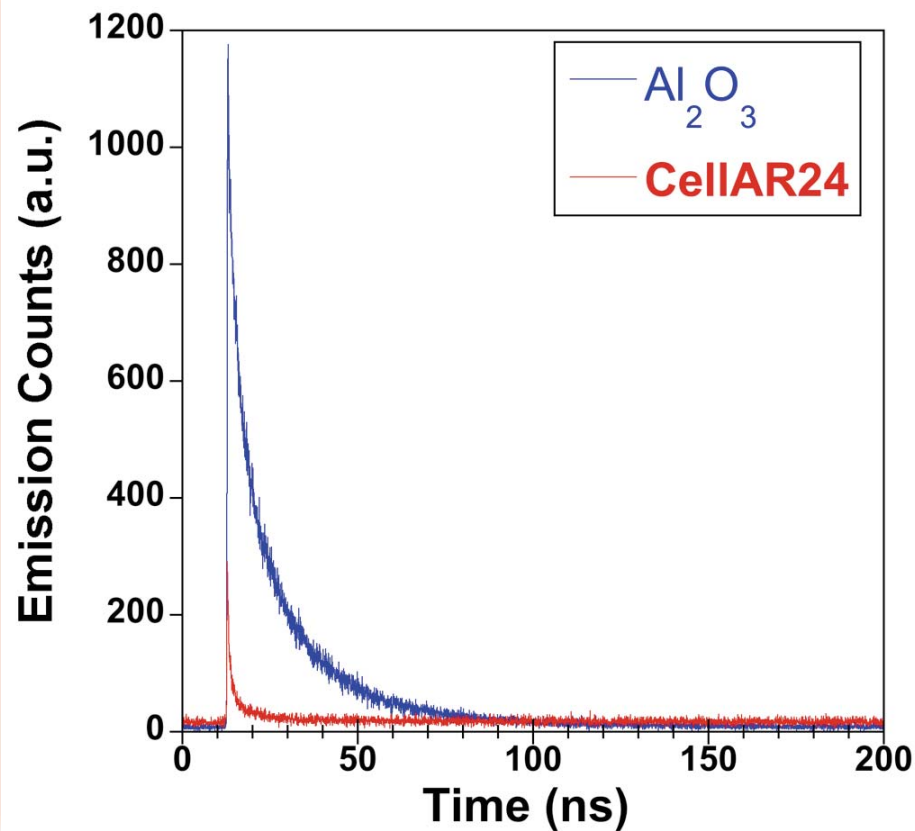


MO



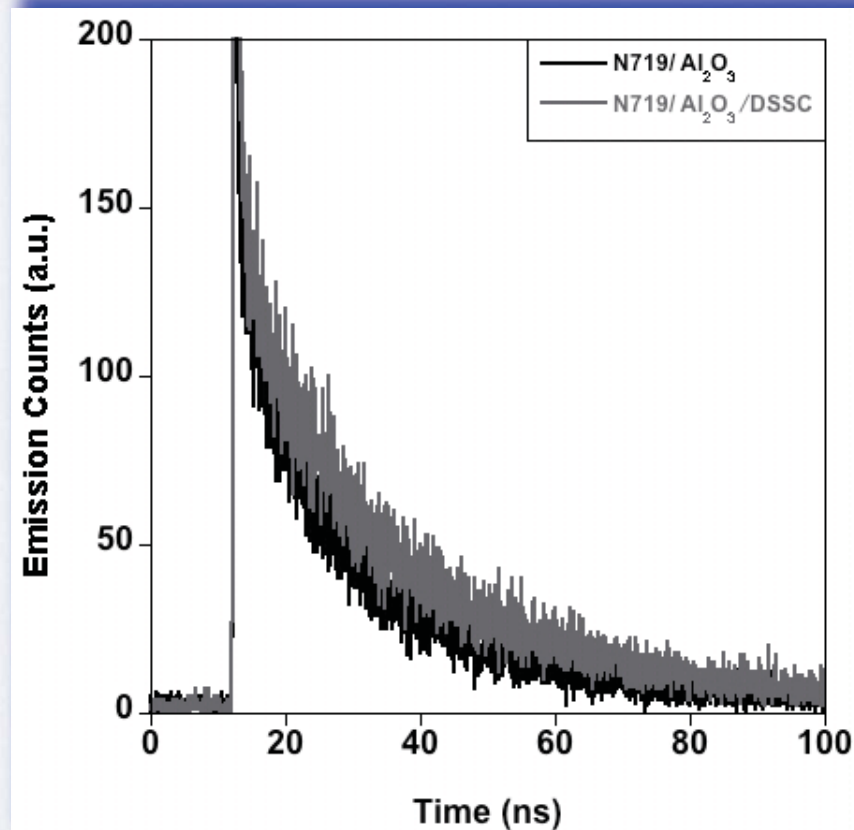
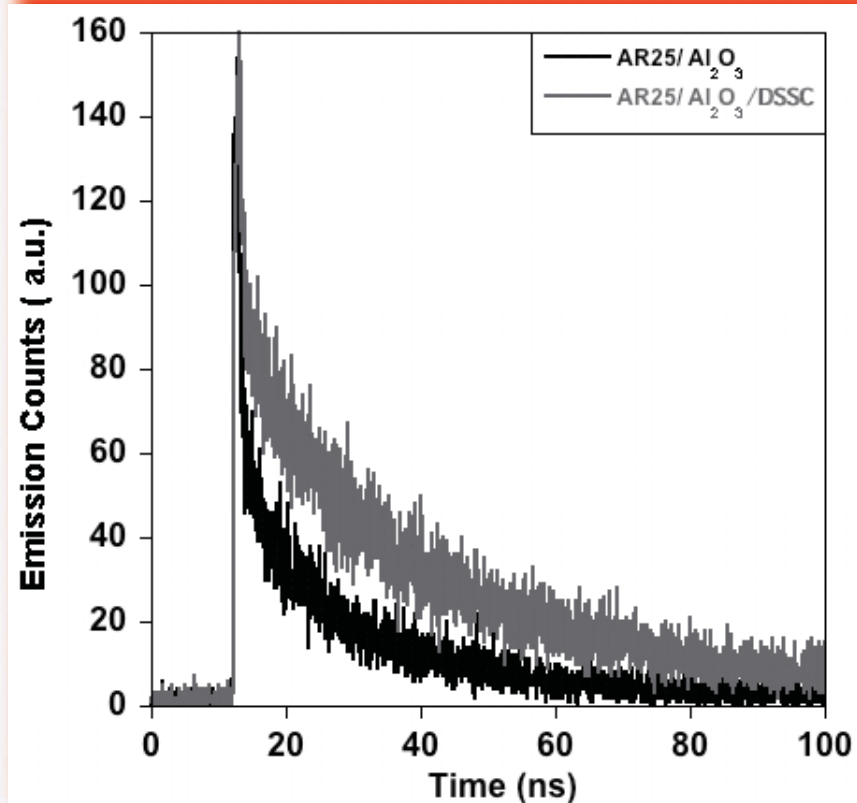
Dye Sensitised Solar Cells

Electron Injection



Dye Sensitised Solar Cells

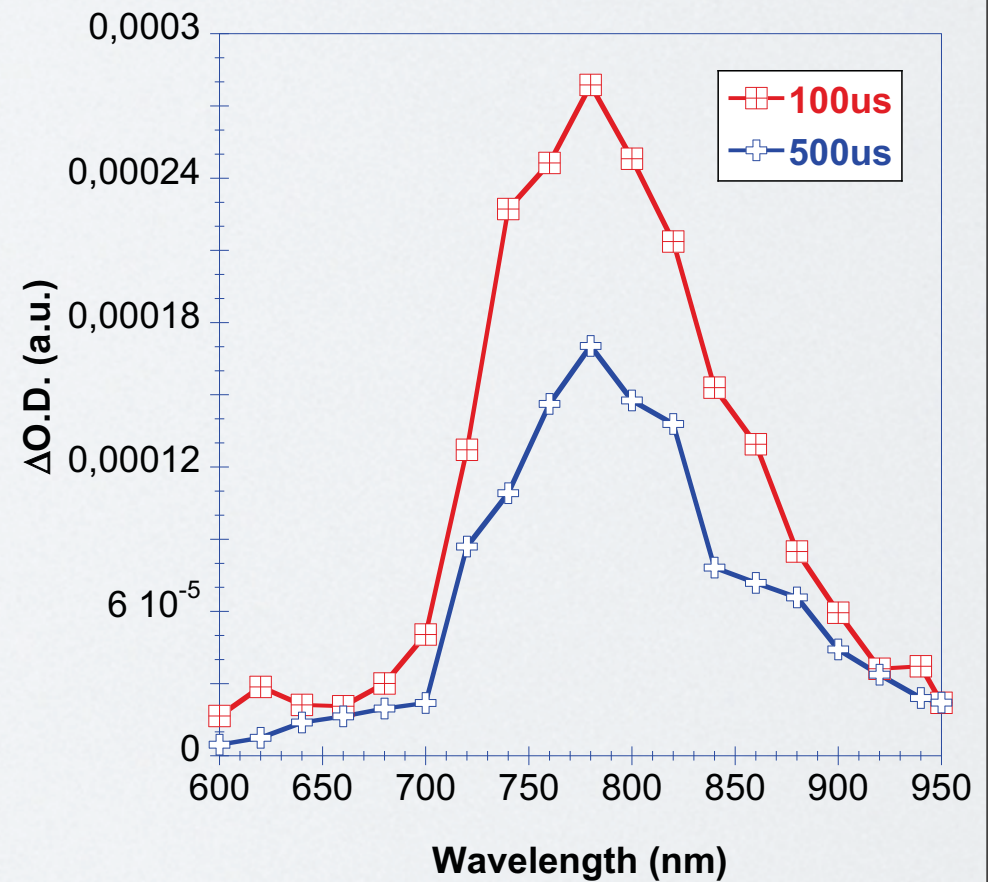
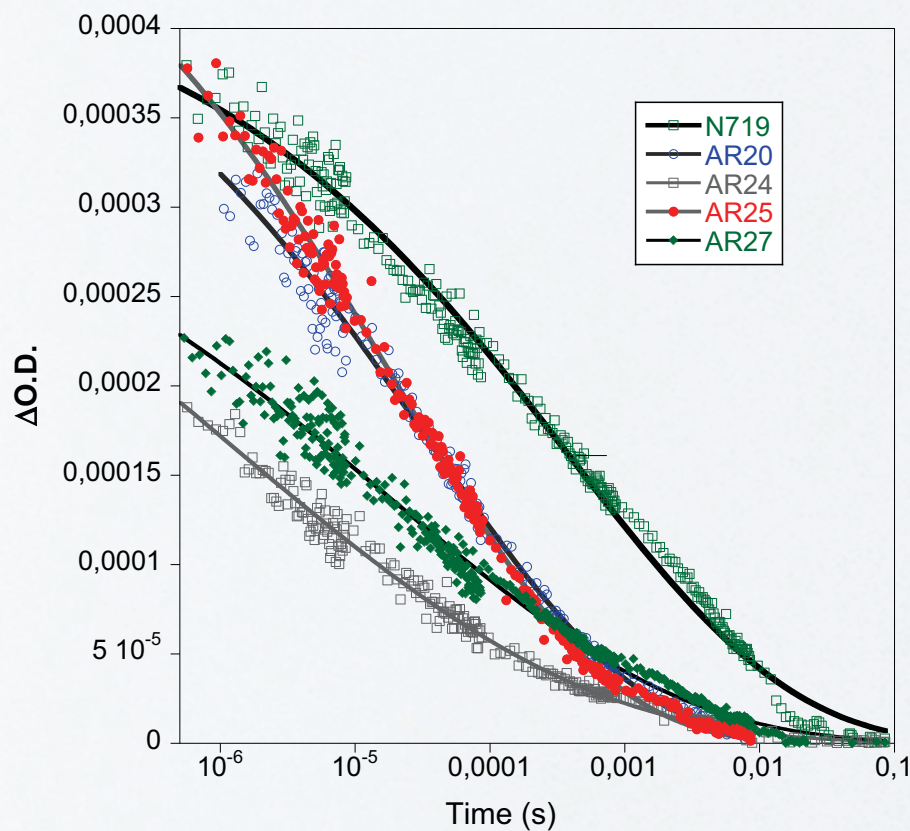
Electron Injection



Dye Sensitised Solar Cells



e^- -TiO₂/Dye⁺ Recombination

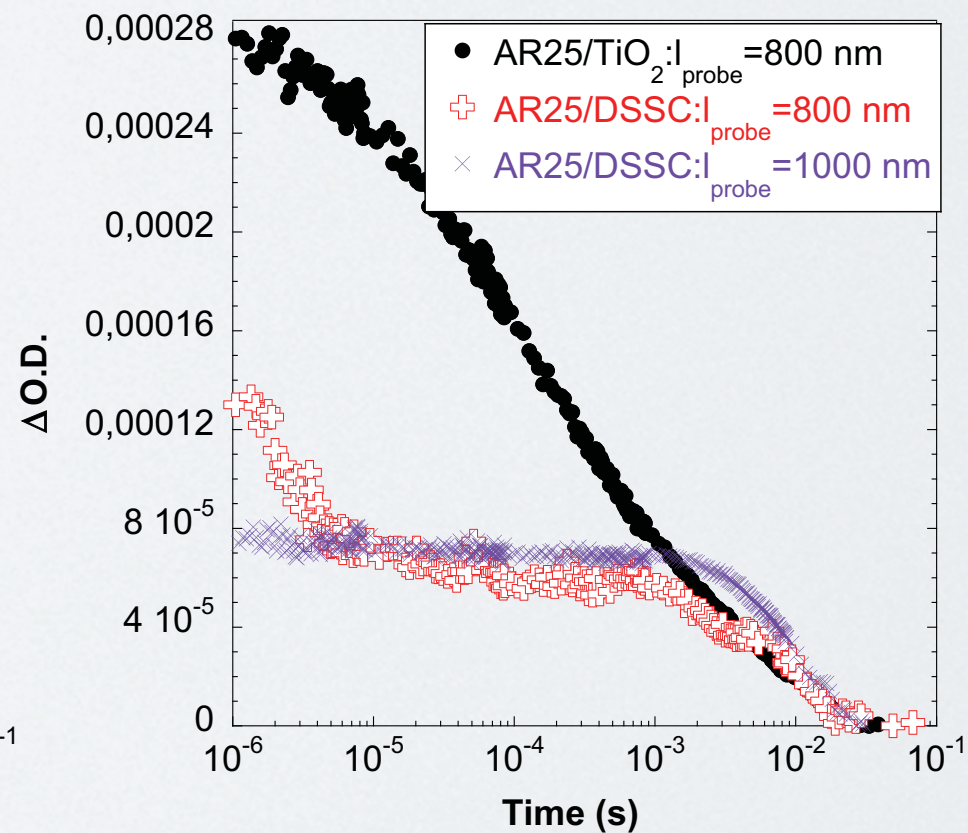
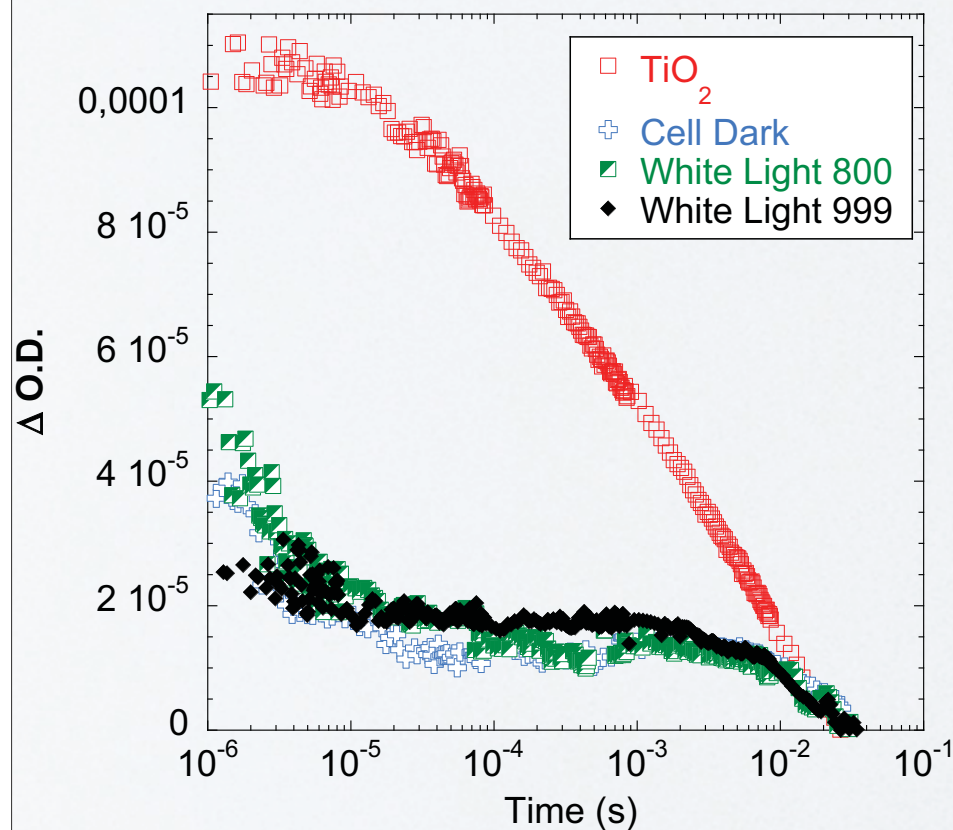


Dye Sensitised Solar Cells



e^- -TiO₂/Dye⁺ Recombination

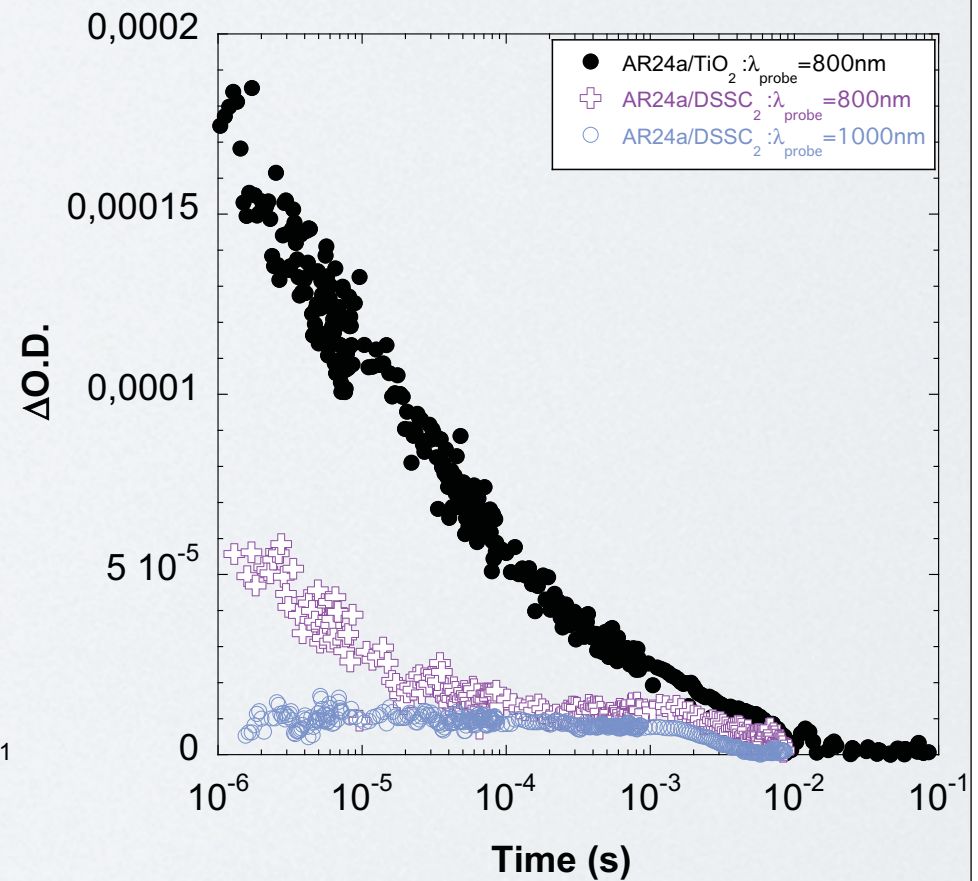
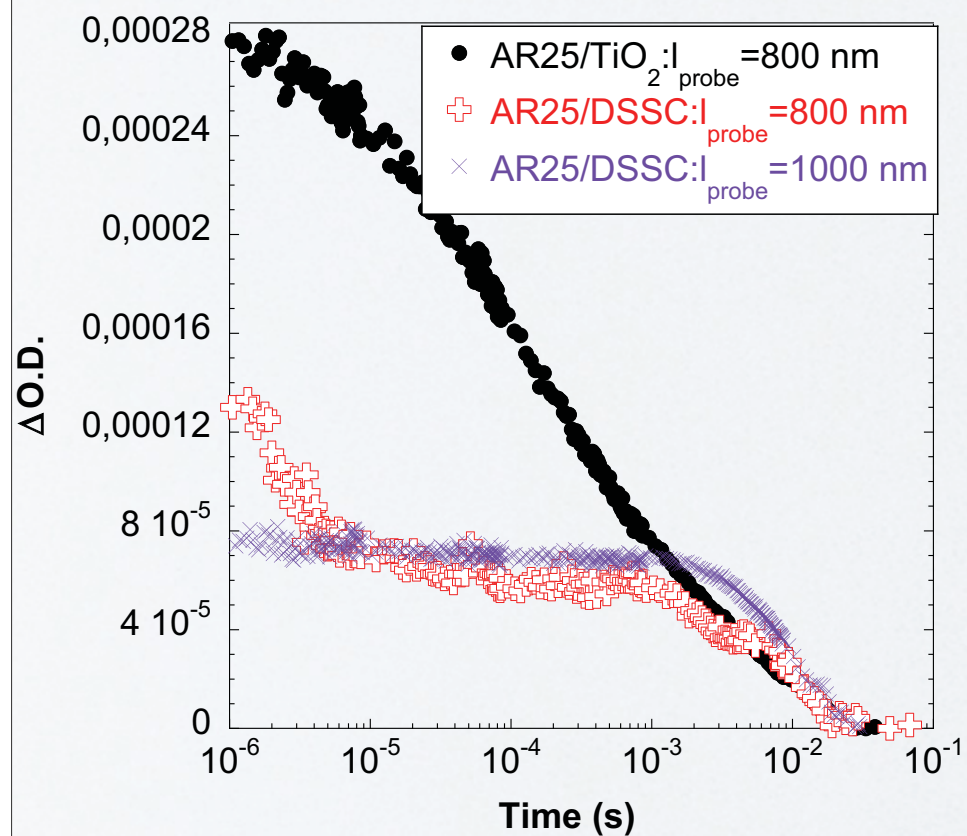
N719



Dye Sensitised Solar Cells



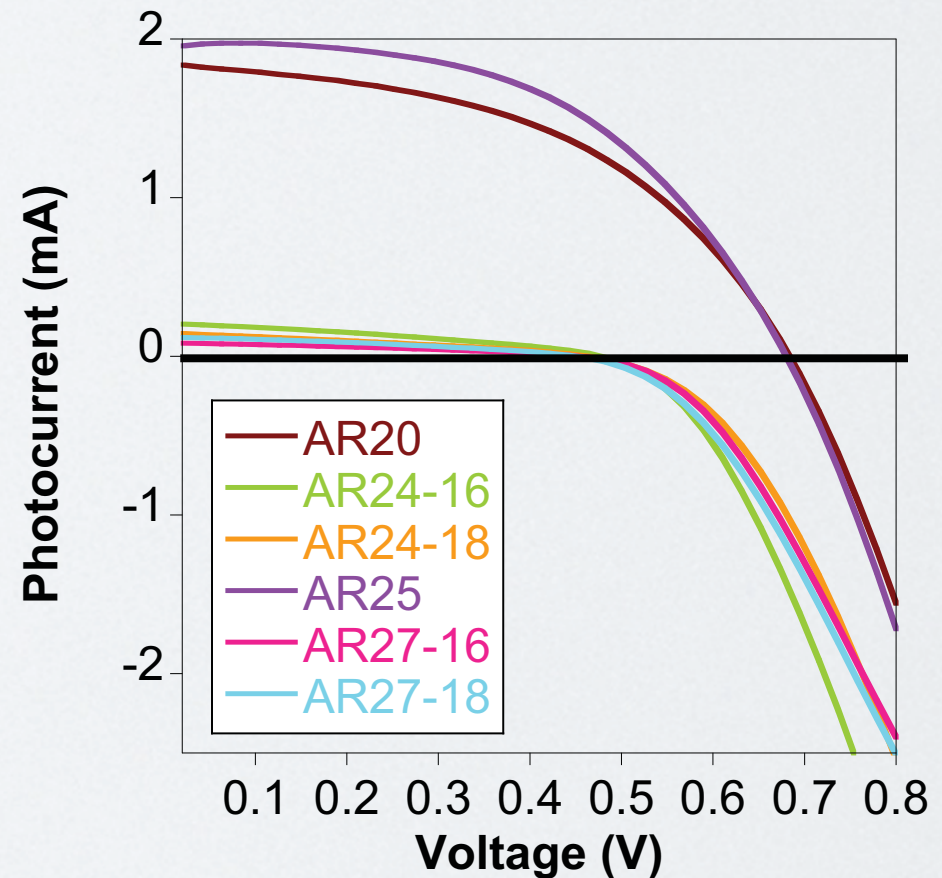
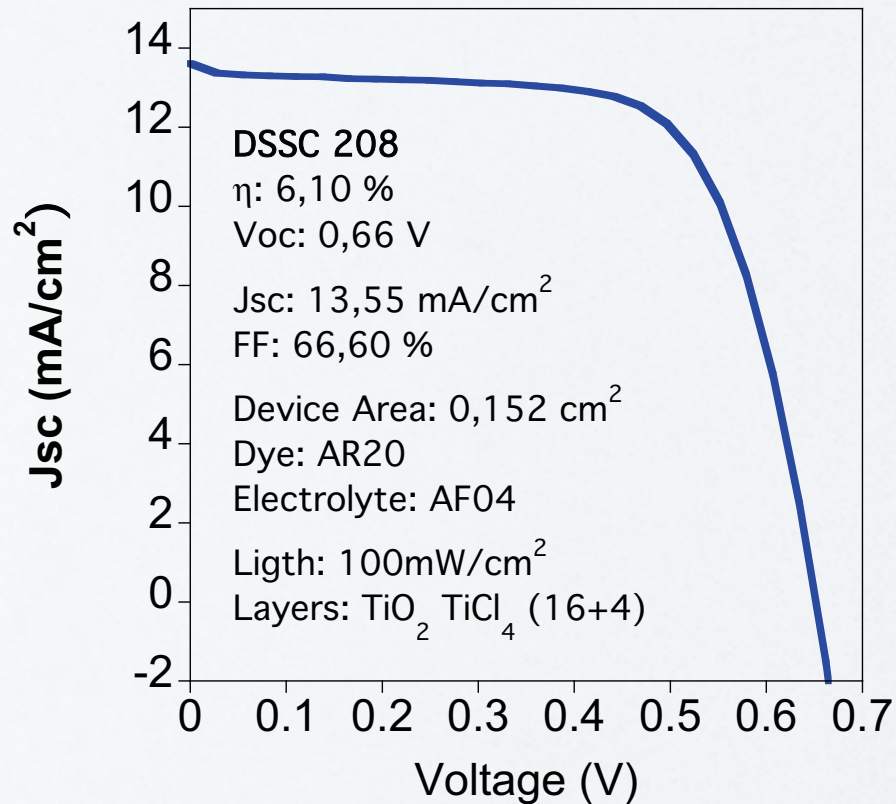
e^- -TiO₂/Dye⁺ Recombination



Dye Sensitised Solar Cells

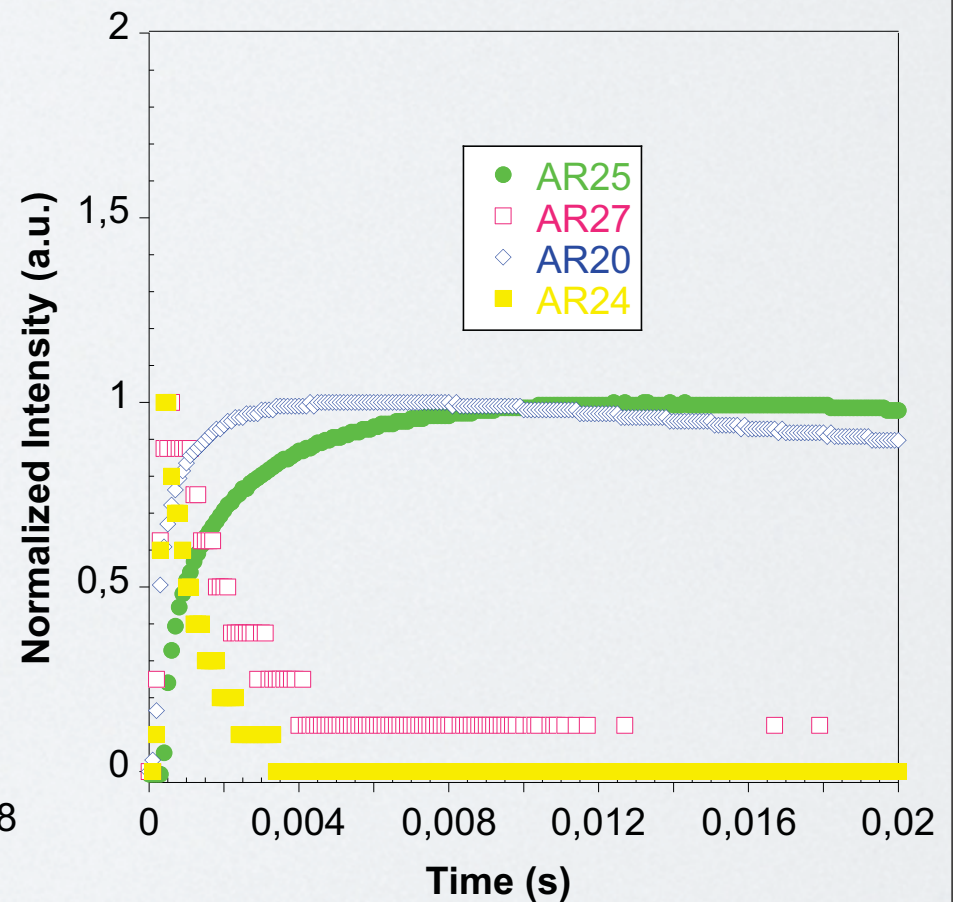
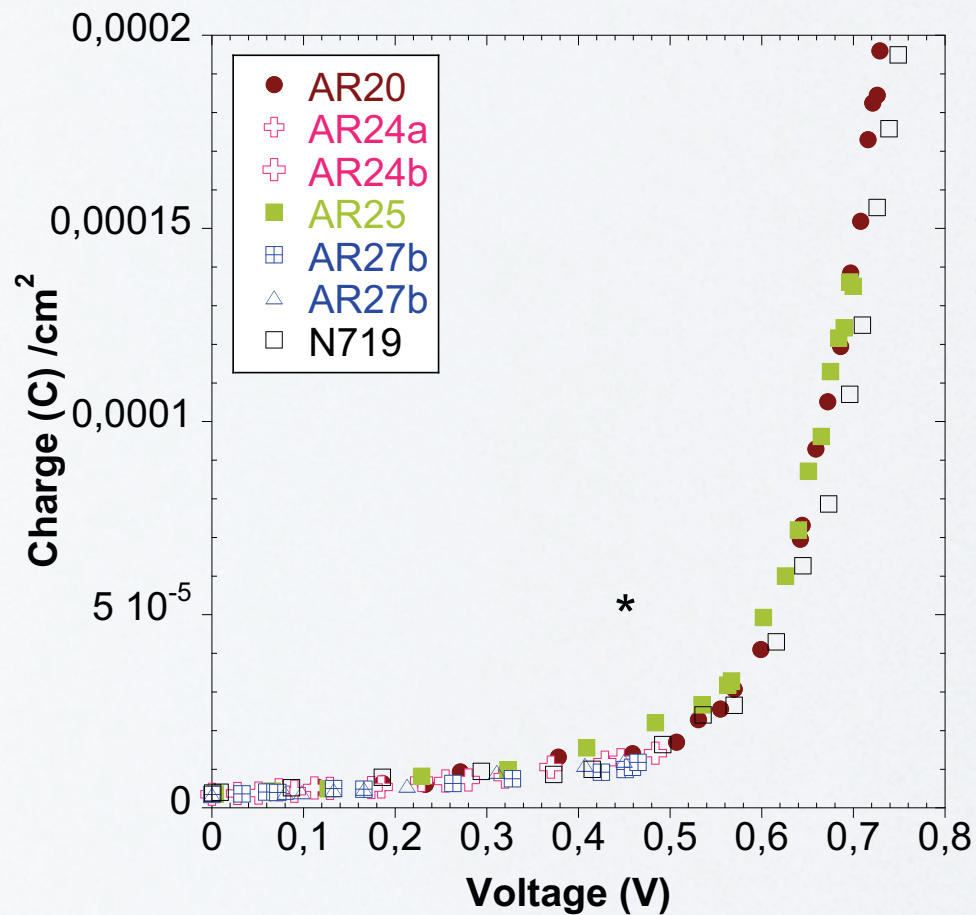


Cell Characterisation



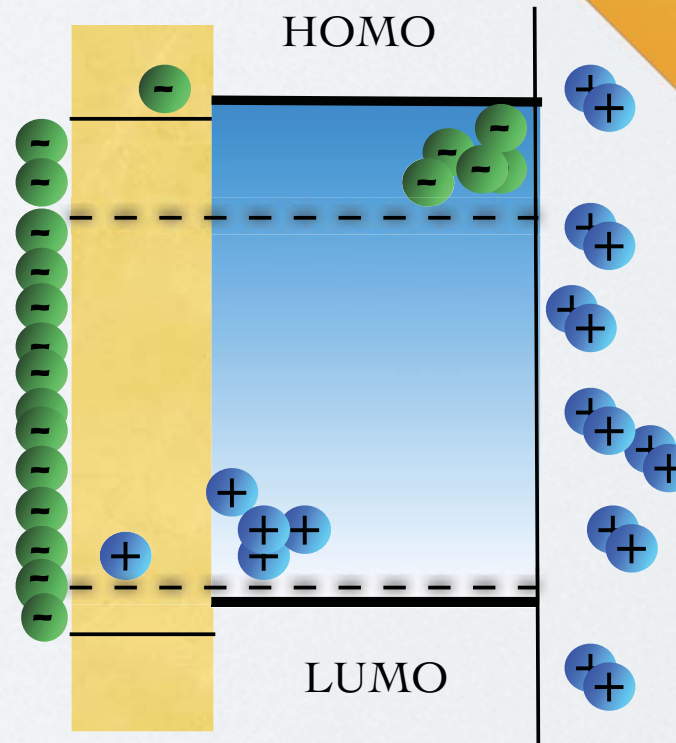
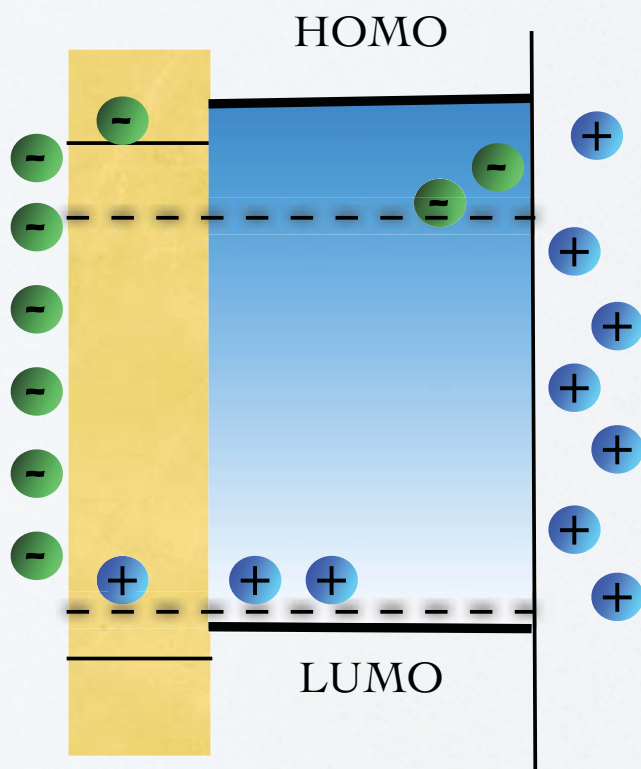
Dye Sensitised Solar Cells

 e^- -TiO₂/Electrolyte⁺ Recombination





Organic solar cells

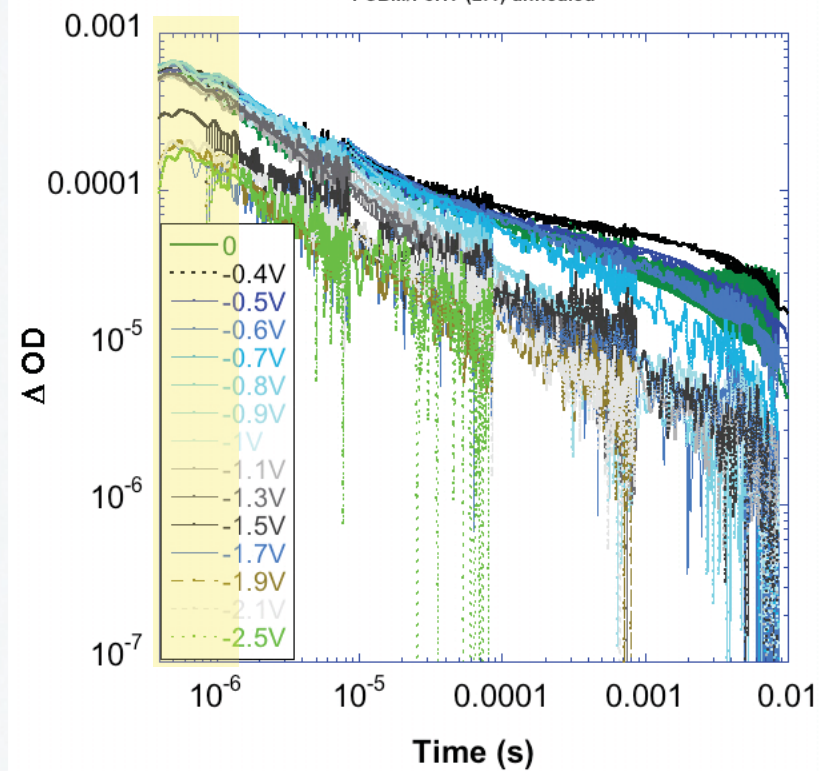




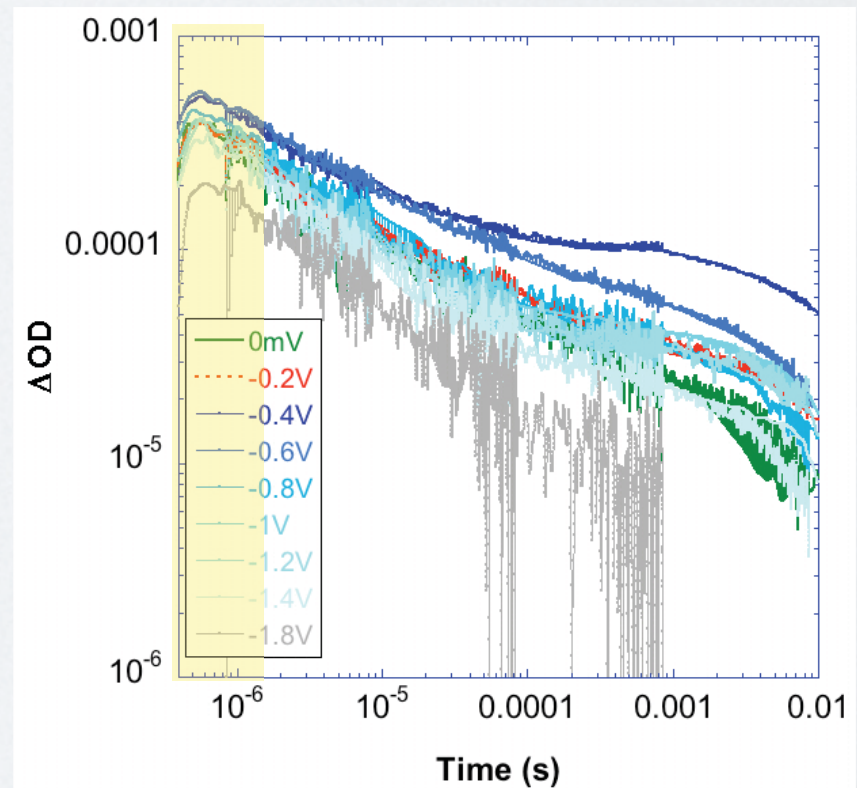
Organic solar cells

P3HT/PCBM

PCBM/P3HT (2:1) annealed



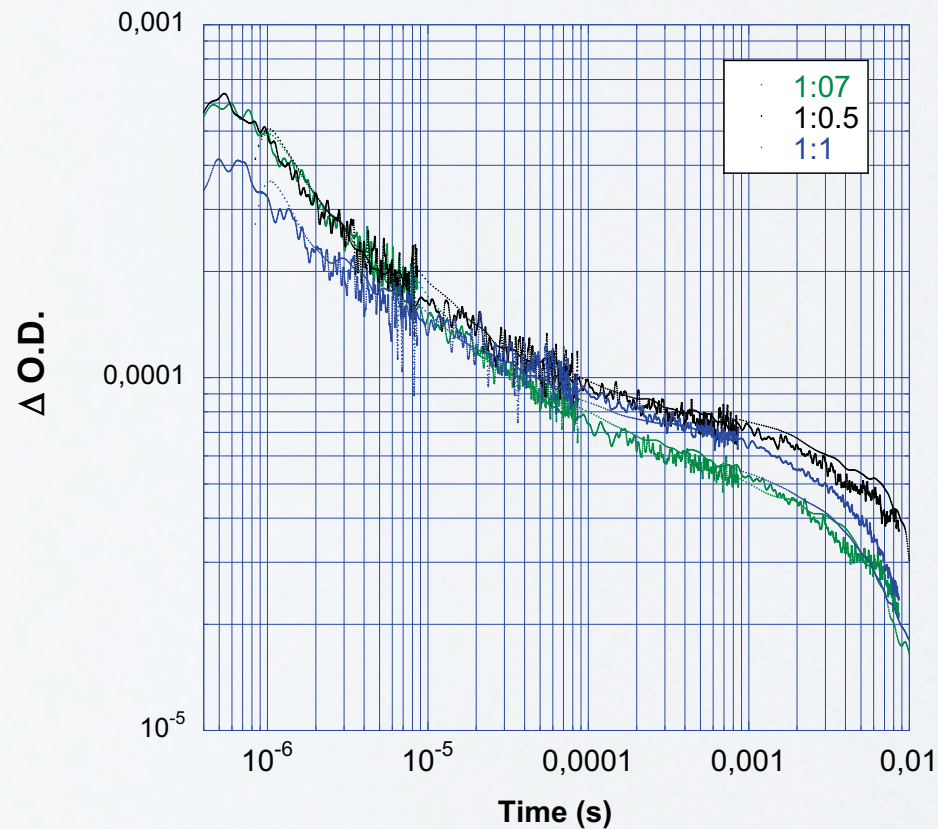
d-TiO₂/ P3HT/PCBM





Organic solar cells

P3HT/PCBM

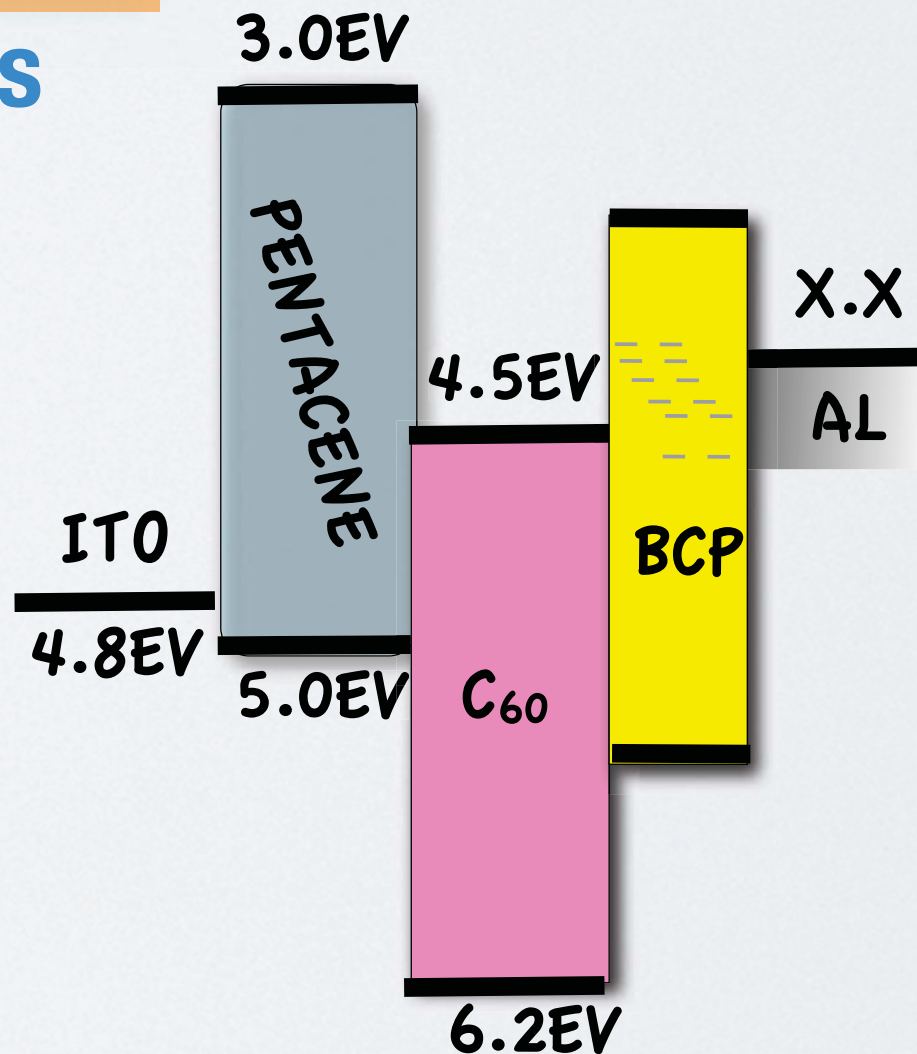
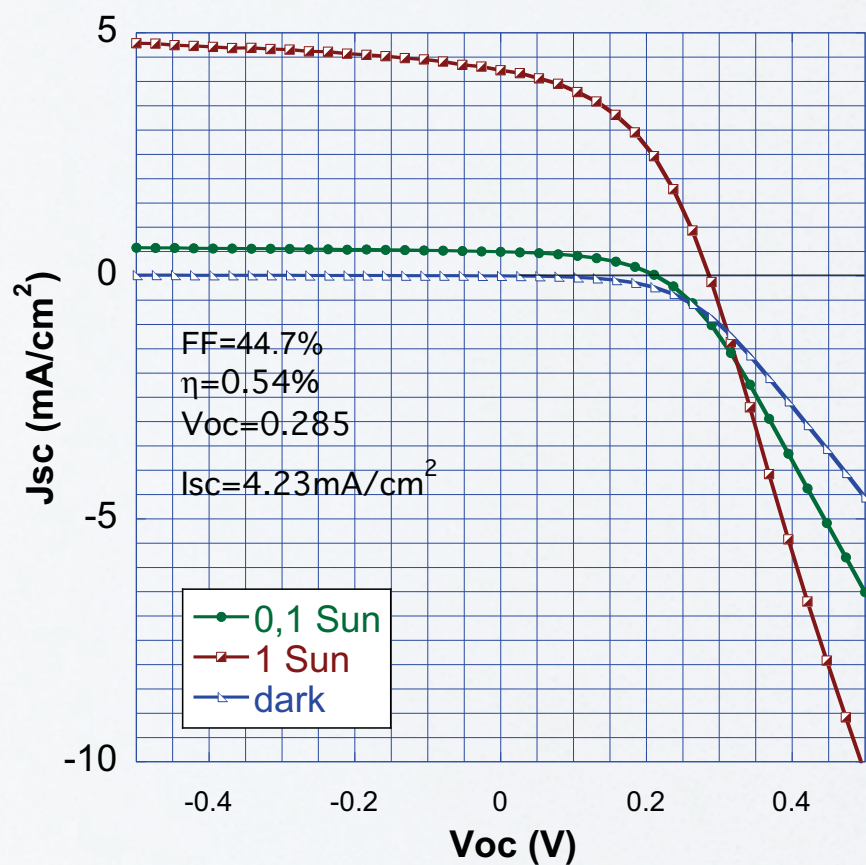


Charge recombination
dynamics
dependent on P3HT/PCBM
ratio



Organic solar cells

ITO/pentacene/C₆₀/BCP/Al

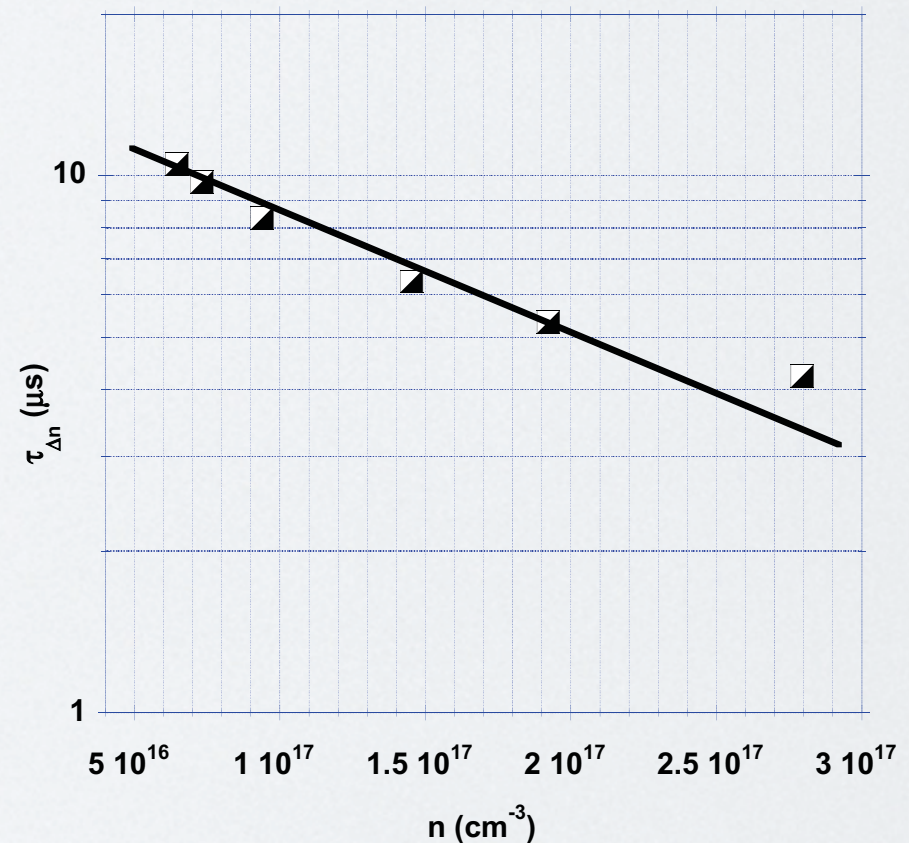
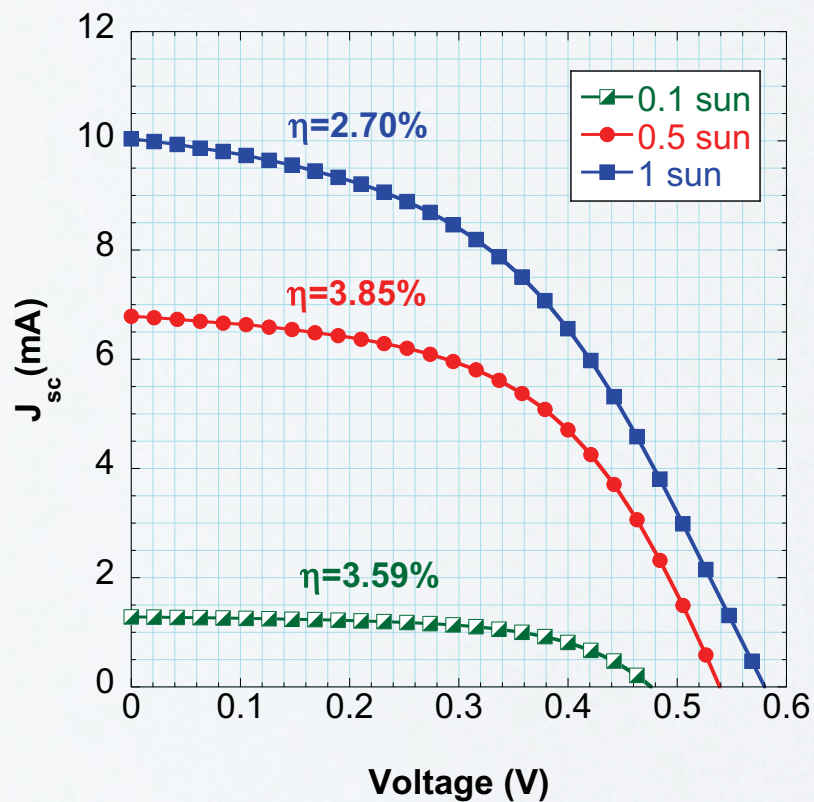




Organic solar cells

ITO/C₆₀: ZnPc/DINPB/NDP2-DiNPB/NDP2-ZnPc/Au/Ag/Au

tau teorico



Acknowledgments

 Research Group Members
and collaborators

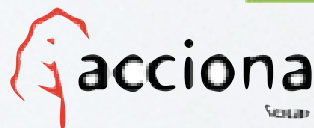
 Funding Agencies



mec.es



 Private Funding



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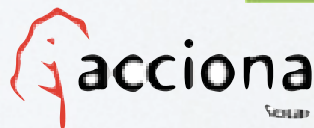
 Funding Agencies



mec.es



 Private Funding



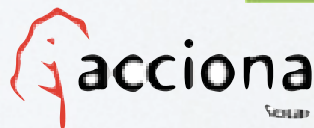
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