A perspective on Organic Photovoltaics

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21st

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

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RENEWABLE AND SUSTAINABLE ENERGY INSTITUTE

Colorado
University of Colorado at Boulder

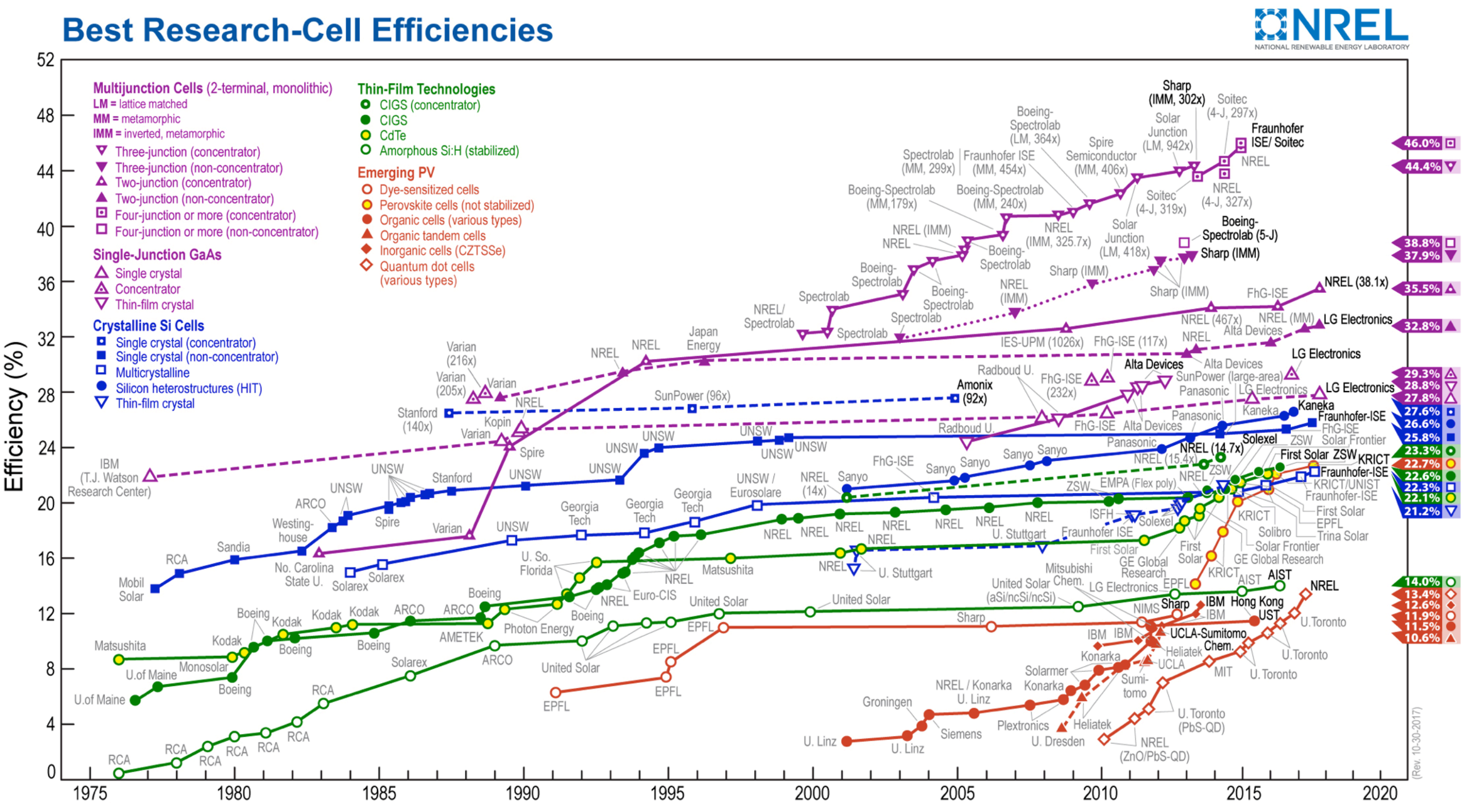
Outline

- Research cell efficiencies
- Driving force for electron transfer and the relationship to V_{oc}
- Charge-Transfer states, Charge-Separated states, and the state of separated charges
- IP, E_A, v E_{ox}, E_{red}

Funding by the Solar Photochemistry Program
Division of Chemical Sciences, Geosciences, and Biosciences

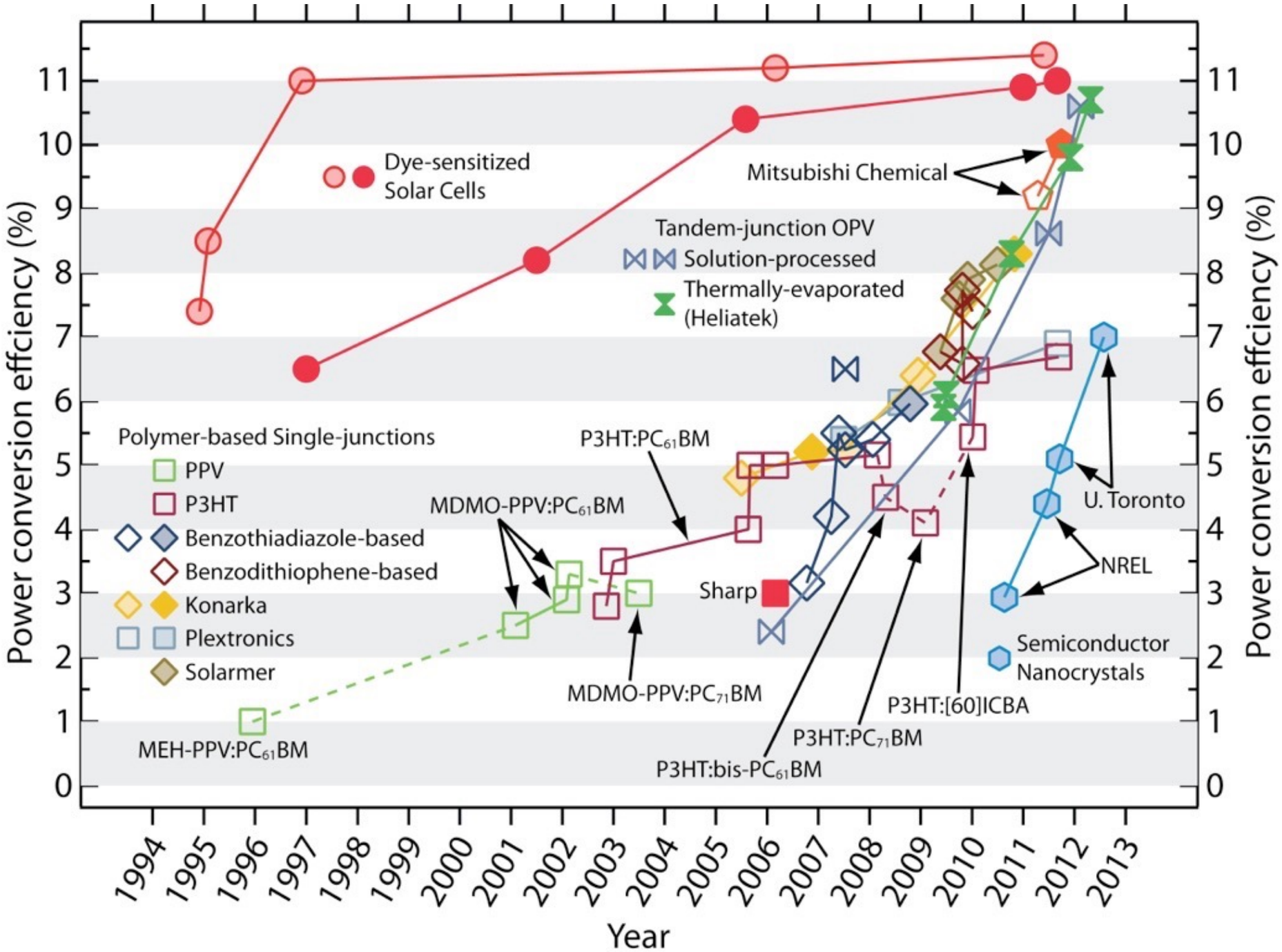
U.S. DEPARTMENT OF ENERGY | Office of Science

Tracking Research Cell Progress



NREL efficiency chart (https://www.nrel.gov/pv/assets/images/efficiency-chart.png)

Tracking Research Cell Progress



[IEEE Spectrum (spectrum.ieee.org/static/interactive-record-breaking-pv-cells)](spectrum.ieee.org/static/interactive-record-breaking-pv-cells)

Interactive: Record-Breaking PV Cells

The world's leading PV research labs use this chart to track record-breaking solar cells. New champs appear as soon as they are certified

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There's often a lot of hype when solar companies claim to set new records. But to see how different PV technologies really stack up, it's important to compare standardized and independent efficiency tests. Here, we present the records that have been independently verified by the world's three leading independent labs.

For explanation of the cell types, cell categories, and additional analysis, please see "What Makes a Good PV Technology?"

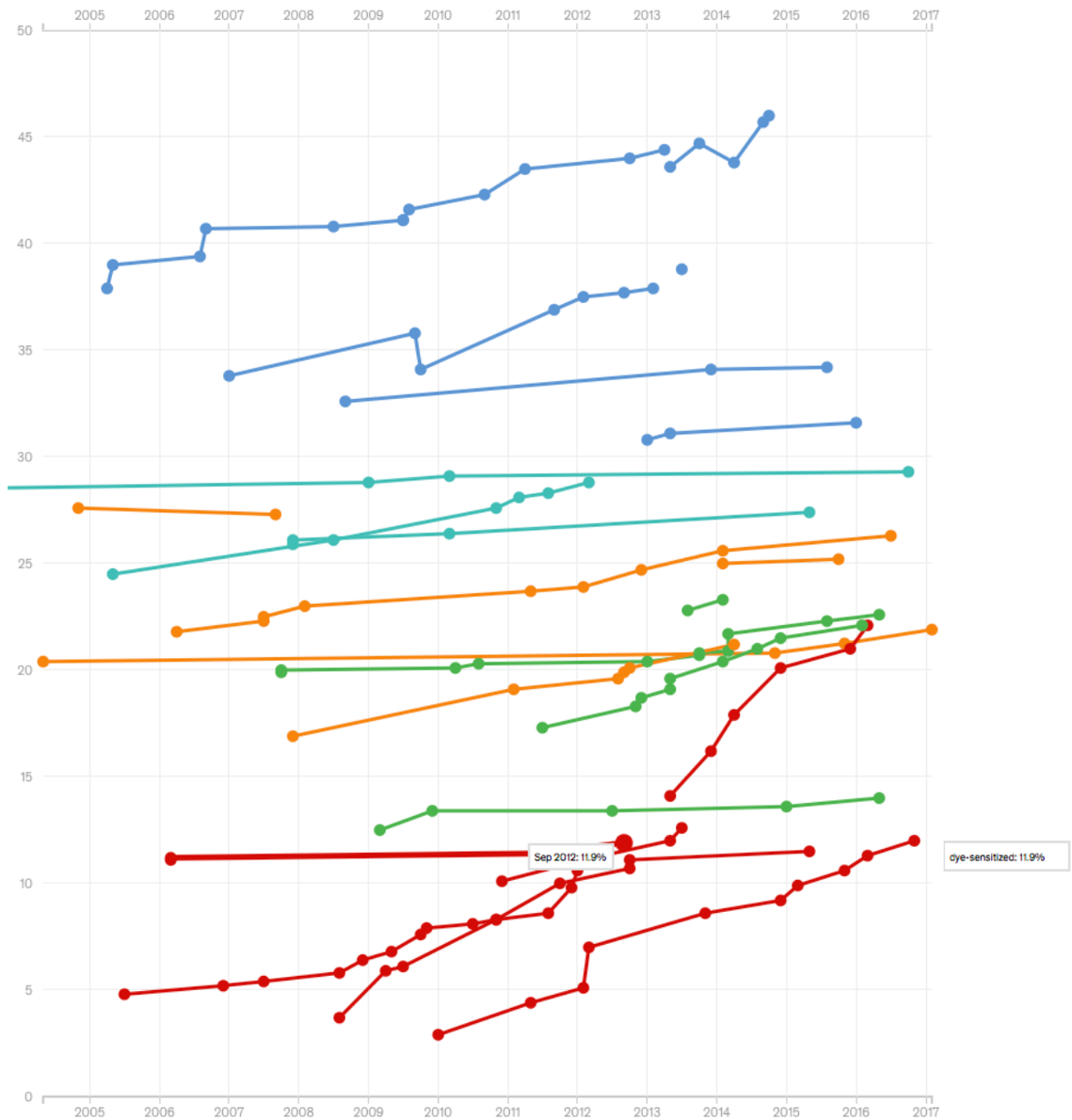
Due to the dense nature of the data, this graphic is best viewed on a large display.

Best Research Cell Efficiencies (Version: 2017-09-21)

Each line on the chart represents a different type of PV cell, and each dot represents a new verified efficiency record. Lines are colored according to the five categories of cells listed below.

● Crystalline Si Cells ● Emerging PV ● Multijunction Cells ● Single-junction GaAs ● Thin-film Technologies

Click any dot to see the detailed information about that record.



Credit: IEEE Spectrum/NREL. Infographic: Josh Romero

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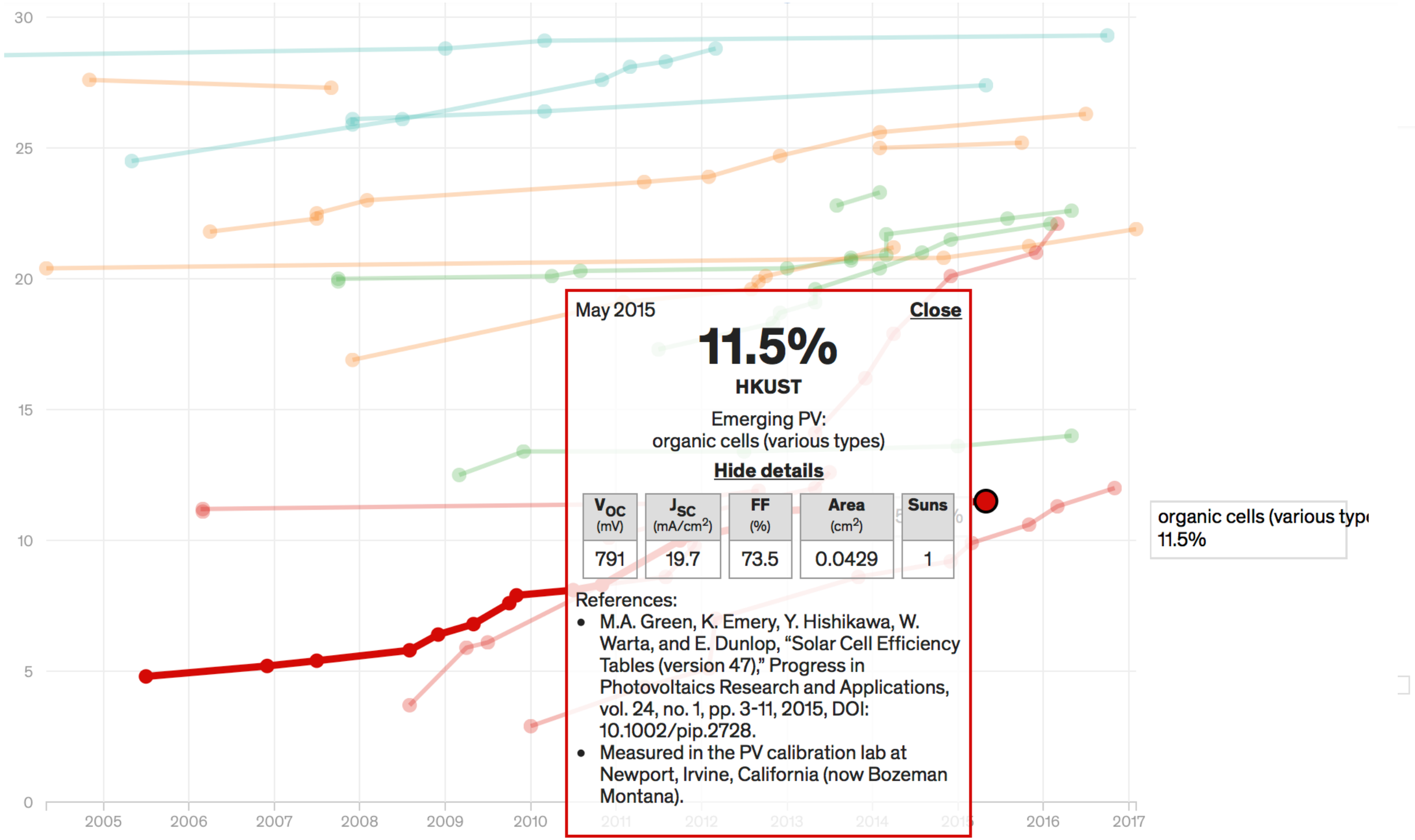

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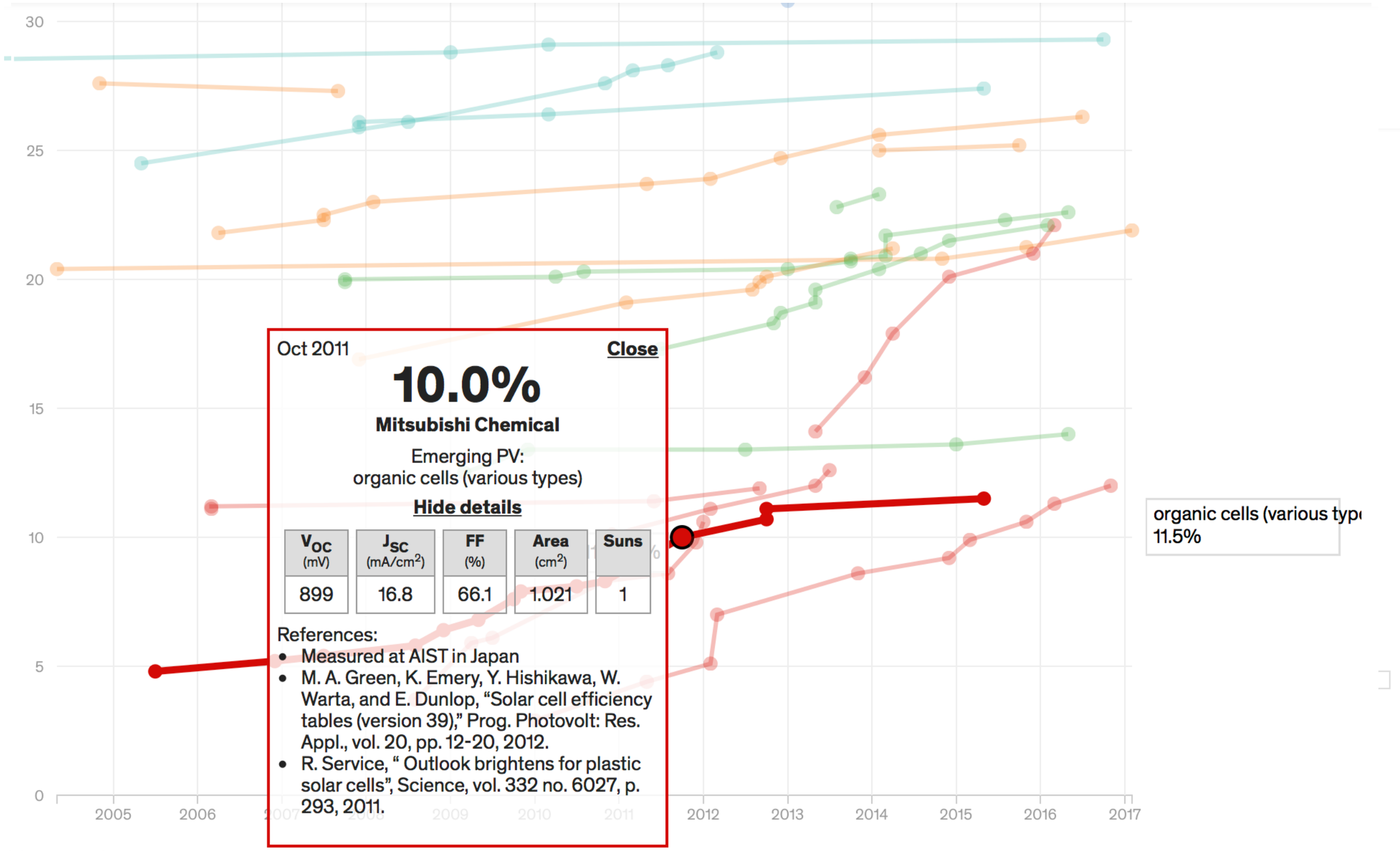

Credit: IEEE Spectrum/NREL. Infographic: Josh Romero

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WILEY PROGRESS IN PHOTOVOLTAICS

ACCELERATED PUBLICATION

Solar cell efficiency tables (version 51)

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[4] National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, CO 80401, USA

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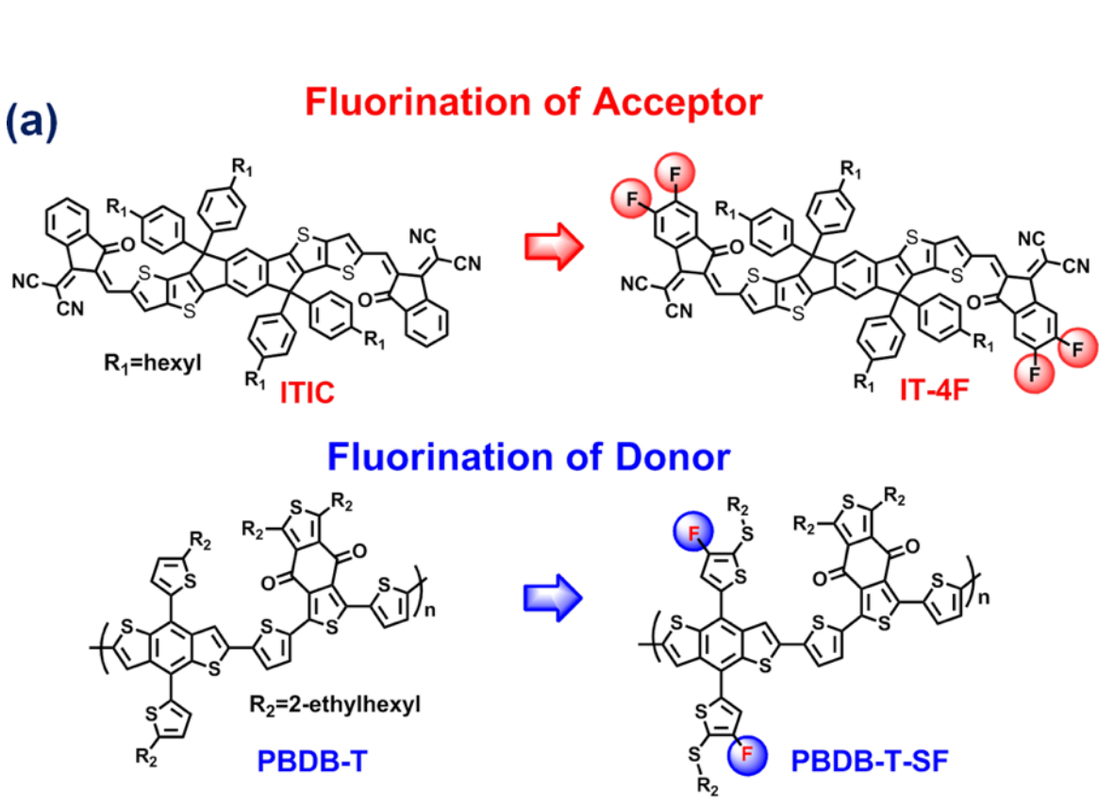
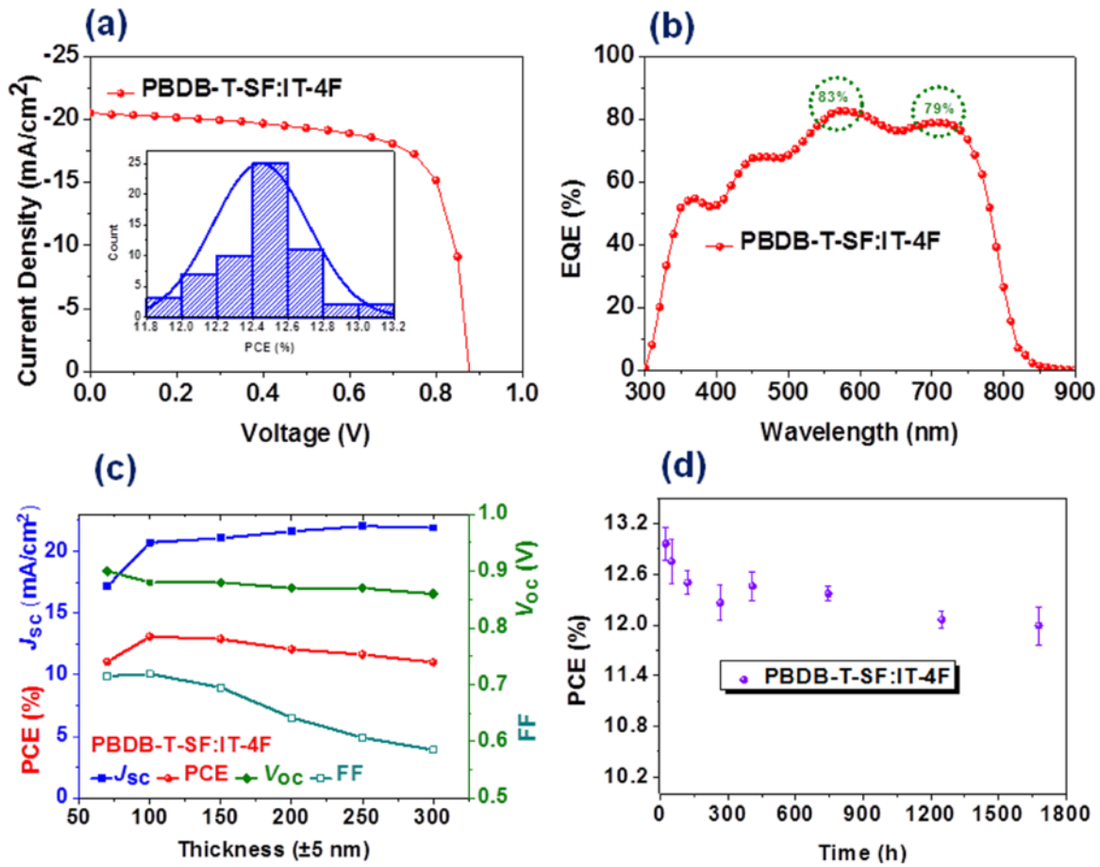
TABLE 4 "Notable exceptions": "Top 10" confirmed cell and module results not class records measured under the global AM1.5 spectrum (1000 Wm^{-2}) at 25°C (IEC 60904-3: 2008, ASTM G-173-03 global)

Classification	Efficiency, %	Area, cm^2	V_{oc}, V	J_{sc}, mA/cm^2	Fill Factor, %	Test Centre (date)	Description
Cells (silicon)							
Si (crystalline)	25.0 ± 0.5	4.00 (da)	0.706	42.7[a]	82.8	Sandia (3/99)[b]	UNSW p-type PERC top/rear contacts[37]
Si (crystalline)	**25.8 ± 0.5[c]**	**4.008 (da)**	**0.7241**	**42.87[d]**	**83.1**	**FhG-ISE (7/17)**	**FhG-ISE, n-type top/rear contacts[38]**
Si (large)	26.6 ± 0.5	179.74 (da)	0.7403	42.5[e]	84.7	FhG-ISE (11/16)	Kaneka, n-type rear IBC[3]
Si (multicrystalline)	**22.0 ± 0.4**	**245.83 (t)**	**0.6717**	**40.55[d]**	**80.9**	**FhG-ISE (9/17)**	**Jinko solar, large p-type[39]**
GaInP	21.4 ± 0.3	0.2504 (ap)	1.4932	16.31[f]	87.7	NREL (9/16)	LG electronics, high bandgap[40]
GaInAsP/GaInAs	**32.6 ± 1.4[c]**	**0.248 (ap)**	**2.024**	**19.51[d]**	**82.5**	**NREL (10/17)**	**NREL, monolithic tandem**
Cells (chalcogenide)							
CIGS (thin-film)	22.6 ± 0.5	0.4092 (da)	0.7411	37.76[f]	80.6	FhG-ISE (2/16)	ZSW on glass[41]
CIGSS (cd free)	22.0 ± 0.5	0.512 (da)	0.7170	39.45[f]	77.9	FhG-ISE (2/16)	Solar frontier on glass[10]
CdTe (thin-film)	22.1 ± 0.5	0.4798 (da)	0.8872	31.69[g]	78.5	Newport (11/15)	First solar on glass[42]
CZTSS (thin-film)	12.6 ± 0.3	0.4209 (ap)	0.5134	35.21[h]	69.8	Newport (7/13)	IBM solution grown[43]
CZTS (thin-film)	11.0 ± 0.2	0.2339(da)	0.7306	21.74[e]	69.3	NREL (3/17)	UNSW on glass[12]
Cells (other)							
Perovskite (thin-film)	**22.7 ± 0.8[i]**	**0.0935 (ap)**	**1.144**	**24.92[d]**	**79.6**	**Newport (7/17)**	**KRICT[15]**
Organic (thin-film)	12.1 ± 0.3[k]	0.0407 (ap)	0.8150	20.27[e]	73.5	Newport (2/17)	Phillips 66

Non-fullerene acceptors

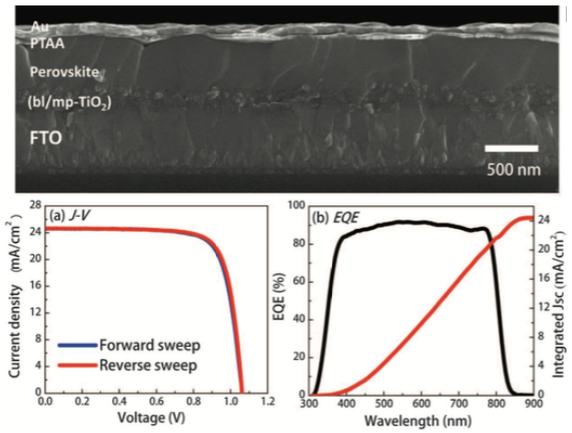
Zhao, W.; Li, S.; Yao, H.; Zhang, S.; Zhang, Y.; Yang, B.; Hou, J.
Molecular Optimization Enables Over 13% Efficiency in Organic Solar Cells.
J Am Chem Soc 2017, 139 (21), 7148–7151.



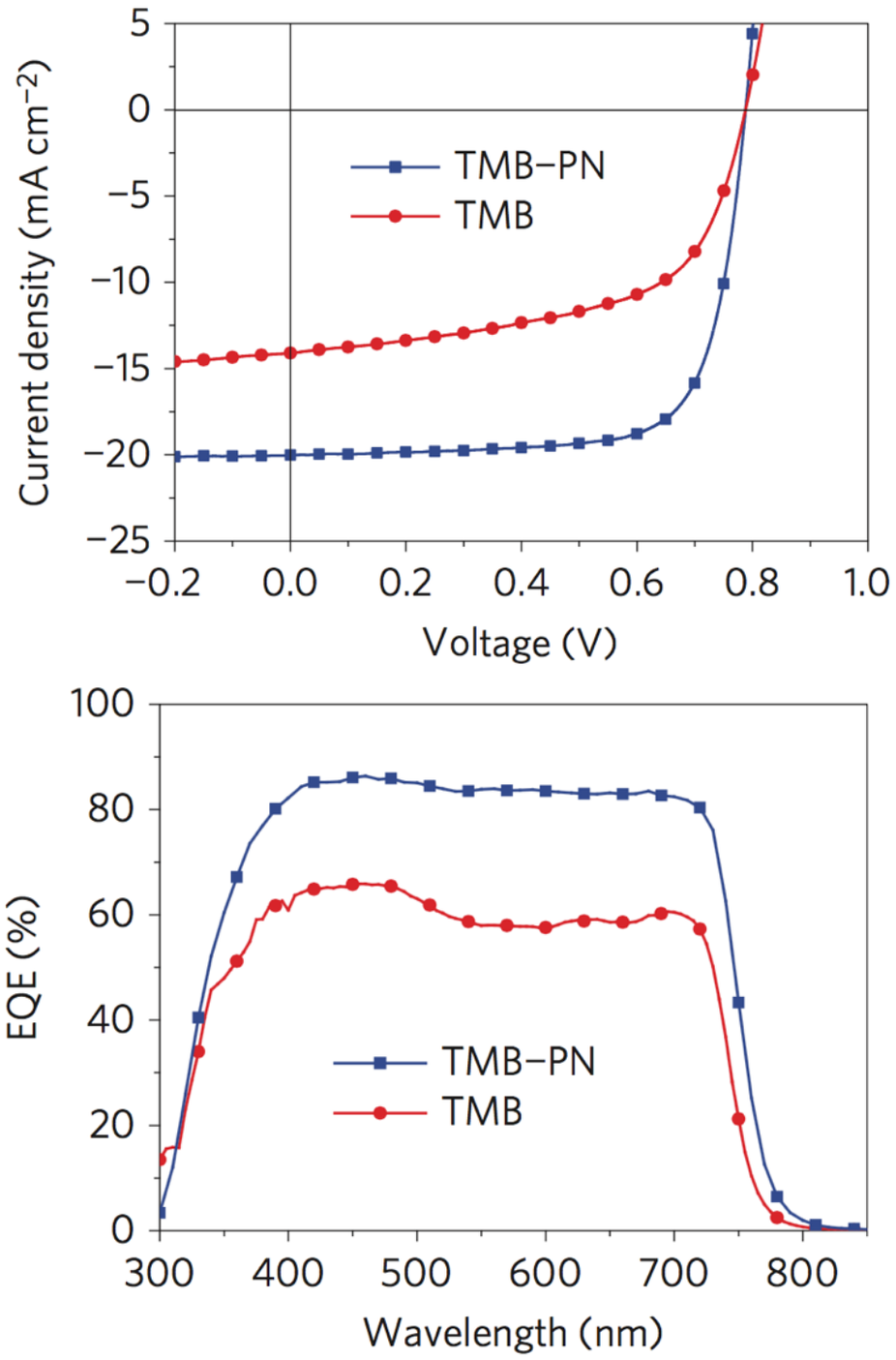


‘Consequently, an impressive PCE of 13.0% was recorded for the PBDB-T-SF:IT-4F-based device, which was certified as 13.1% by the **National Institute of Metrology, China (NIM)**, suggesting that the results obtained in our lab are reliable.’

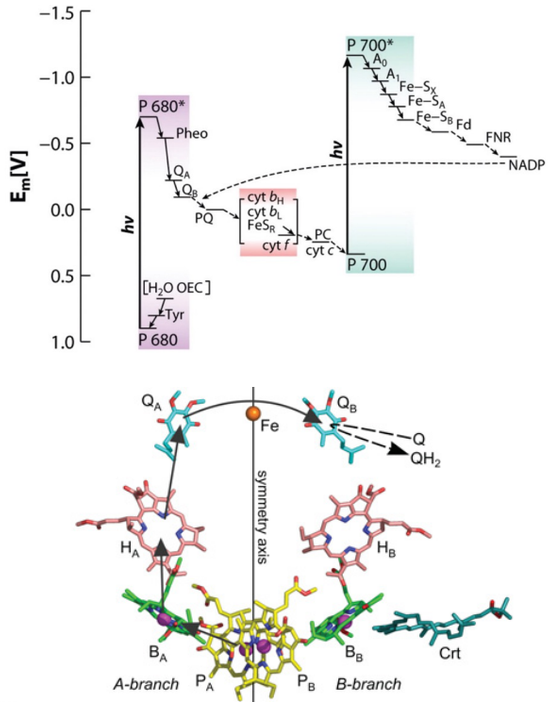
PV: Semiconductors, photosynthesis and organics



Yang, W. S.; Noh, J. H.; Jeon, N. J.; Kim, Y. C.; Ryu, S.; Seo, J.; Seok, S. I.
High-Performance Photovoltaic Perovskite Layers Fabricated Through Intramolecular Exchange.
Science **2015**, 348, 1234–1237.



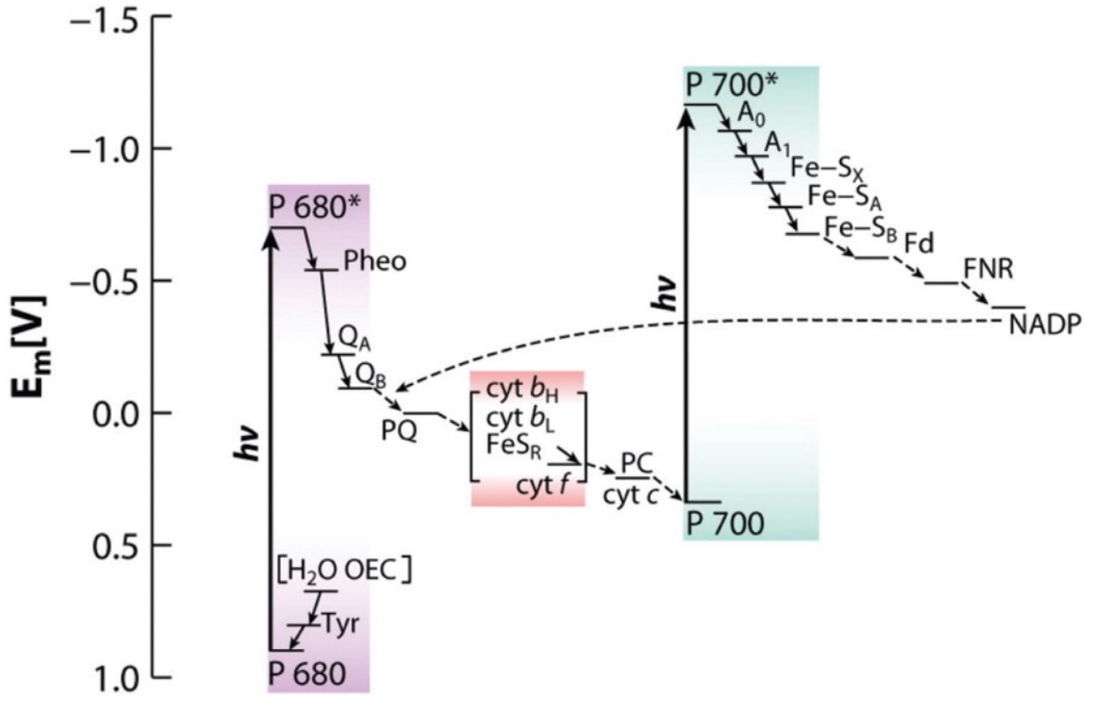
Zhao, J.; Li, Y.; Yang, G.; Jiang, K.; Lin, H.; Ade, H.; Ma, W.; Yan, H.
Efficient Organic Solar Cells Processed From Hydrocarbon Solvents.
Nat. Energy **2016**, 1, 15027.

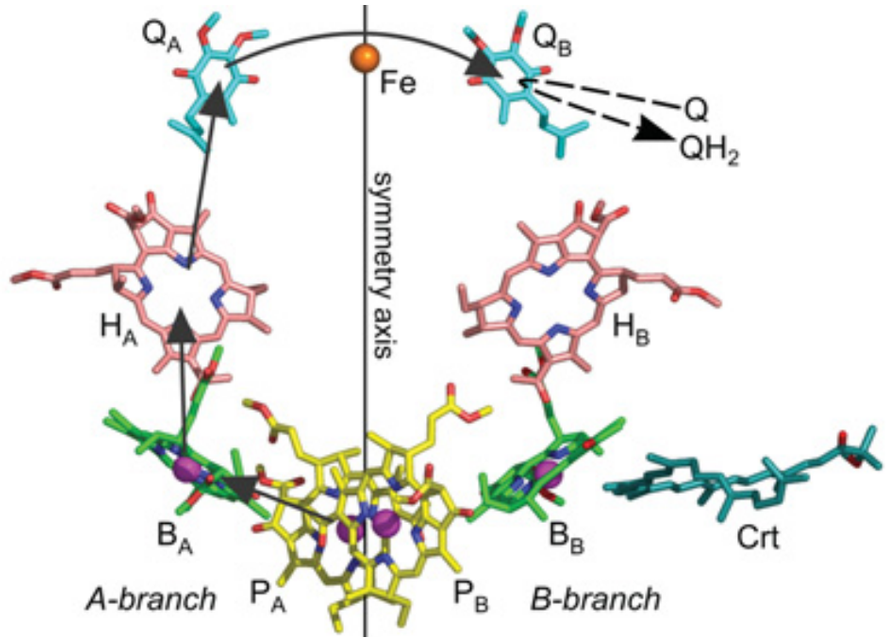


Rhodobacter sphaeroides Reaction Center

Motivation:

- Connect molecular, photo-induced electron transfer theory to the bulk heterojunction solar cell
- Identify role of states intermediate between excitation and free carriers
- Establish the nature of the pathway(s) for recombination
- Understand the role of solid-state microstructure





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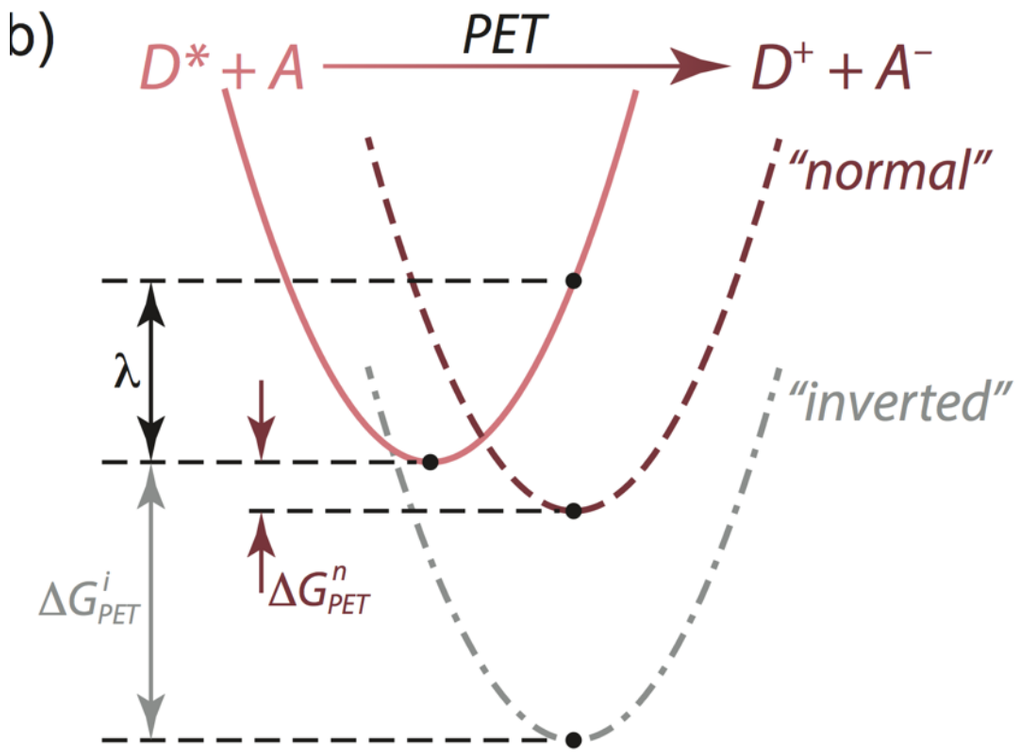
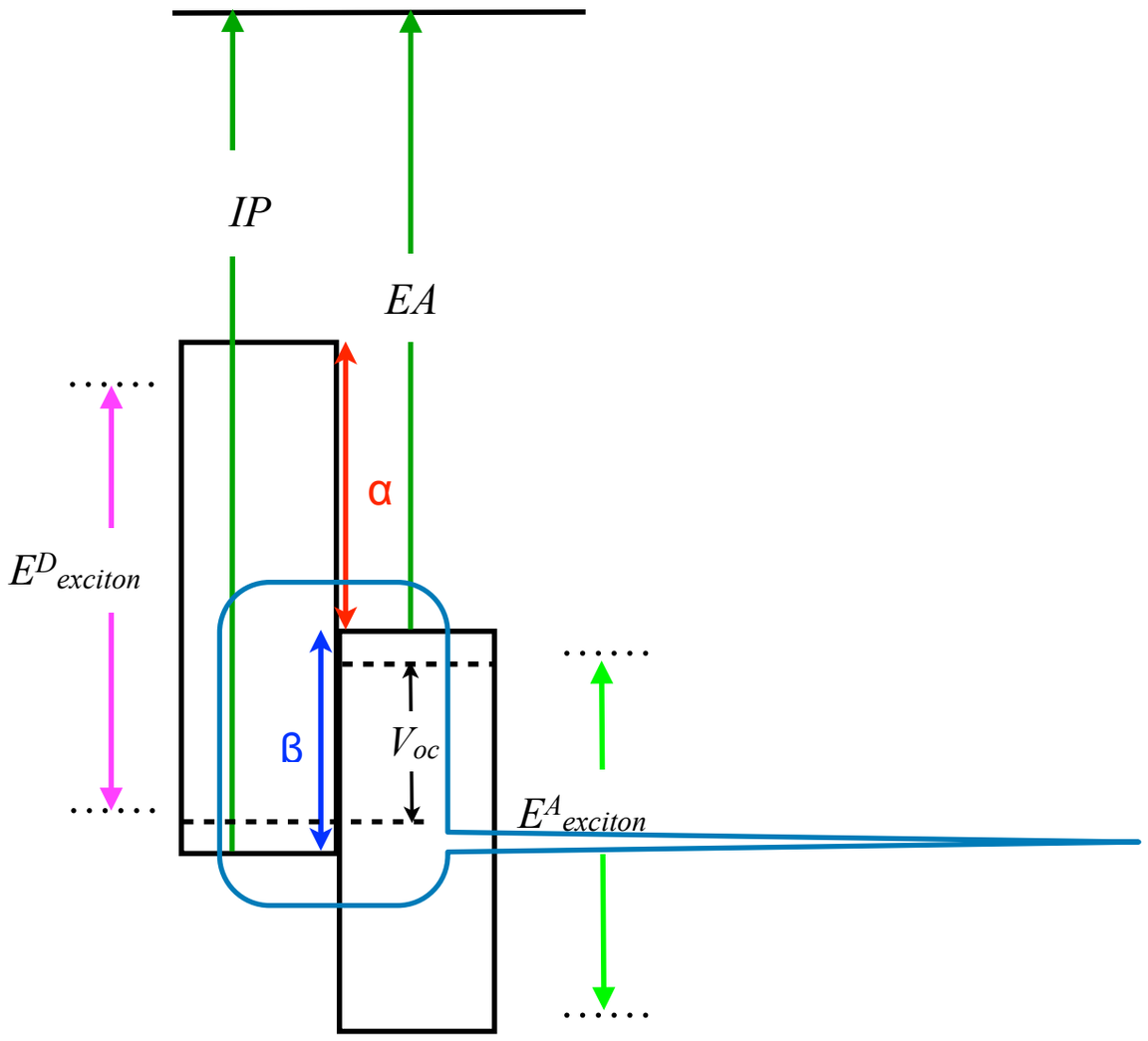


$$k_{ET} = \frac{2\pi}{\hbar}\left|H_{AB}\right|^2 \frac{1}{\sqrt{4\pi\lambda k_B T}} \exp\left(-\frac{\left(\lambda + \Delta G^o\right)^2}{4\lambda k_B T}\right)$$

Why is this important? (Using type II model)



$$\alpha = LUMO_{Acceptor} - LUMO_{Donor}$$

$$\beta = LUMO_{Acceptor} - HOMO_{Donor}$$

$$\approx V_{oc}$$

1. Energy loss associated with exciton dissociation
2. Charge generation mechanism at interface

Exciton* → CS* state / CT* state ⇄ Carriers

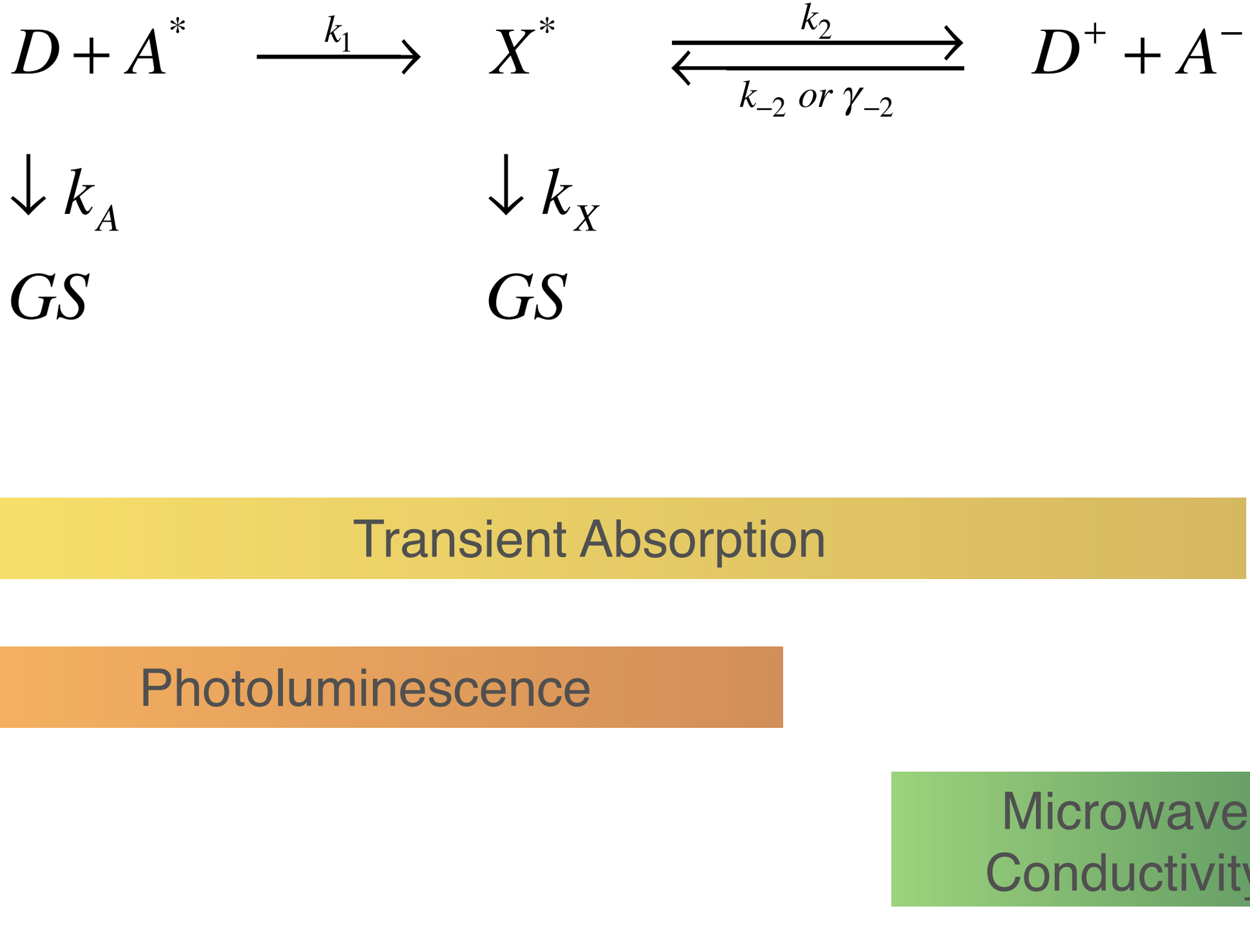
↓

Ground State

Transient Absorption

Photoluminescence

Microwave Conductivity

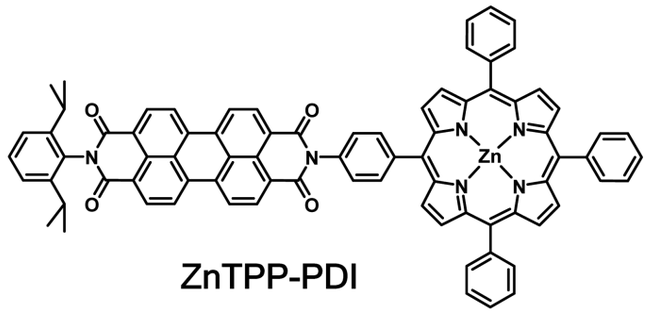


Transient Absorption

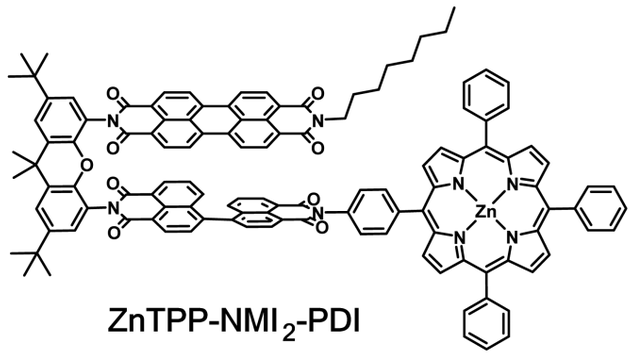
Photoluminescence

Microwave Conductivity

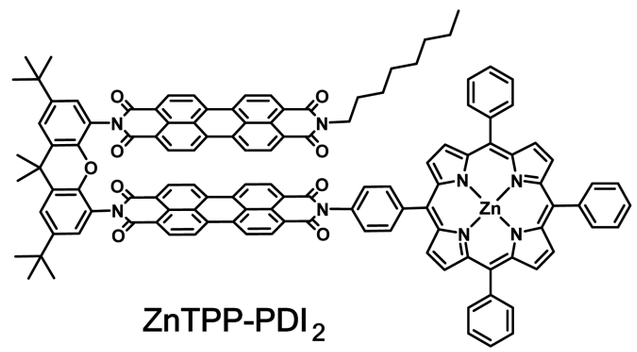
P. E. Hartnett, C. M. Mauck, M. A. Harris, R. M. Young, Y.-L. Wu, T. J. Marks and M. R. Wasielewski, J Am Chem Soc, 2017, jacs.6b10140.



ZnTPP-PDI

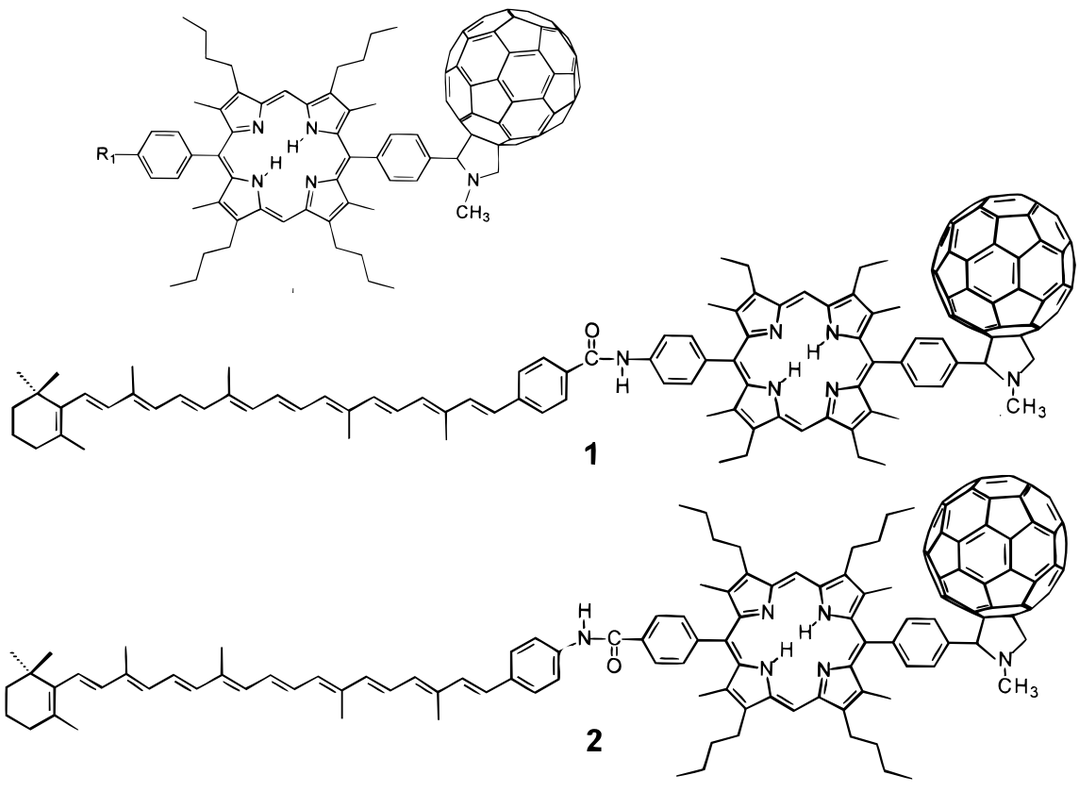


ZnTPP-NMI$_2$-PDI



ZnTPP-PDI$_2$

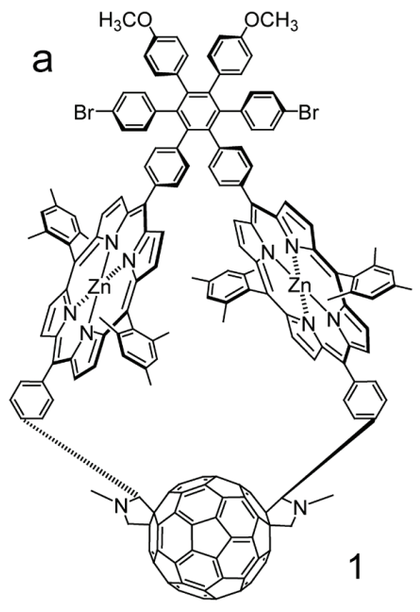
D. Kuciauskas, P. A. Liddell, S. Lin, S. G. Stone, A. L. Moore, T. A. Moore and D. Gust,
J Phys Chem B, 2000, 104, 4307–4321.



1

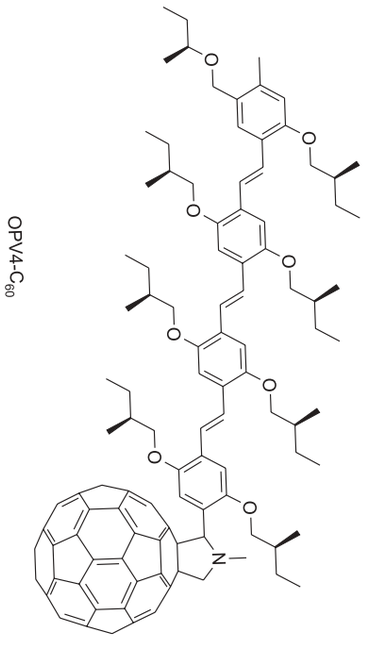
2

V. Garg, G. Kodis, M. Chachisvilis, M. Hambourger, A. L. Moore, T. A. Moore and D. Gust,
J Am Chem Soc, 2011, 133, 2944–2954.



1

P. A. van Hal, S. C. J. Meskers and R. A. J. Janssen,
Appl Phys A-Mater, 2004, 79, 41–46.

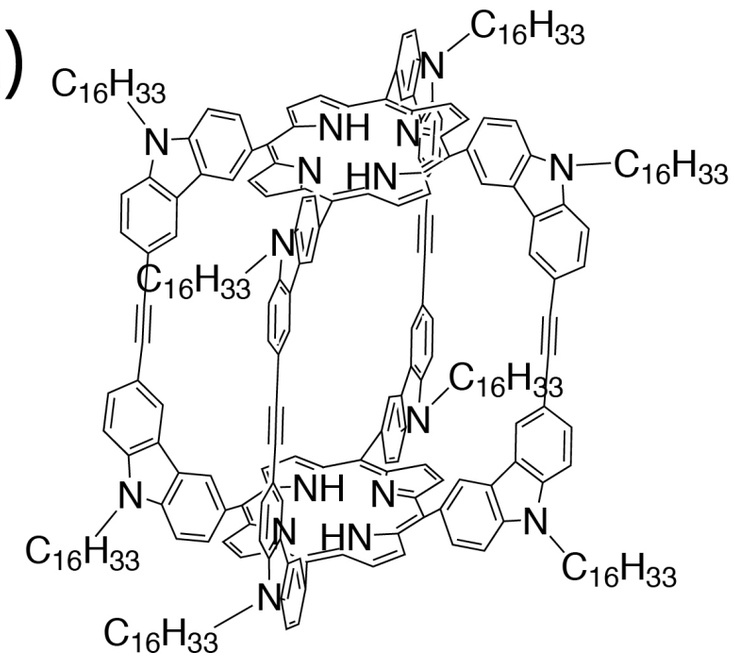


OPV4-C$_{60}$

All in low dielectric constant solvents (<7.6)

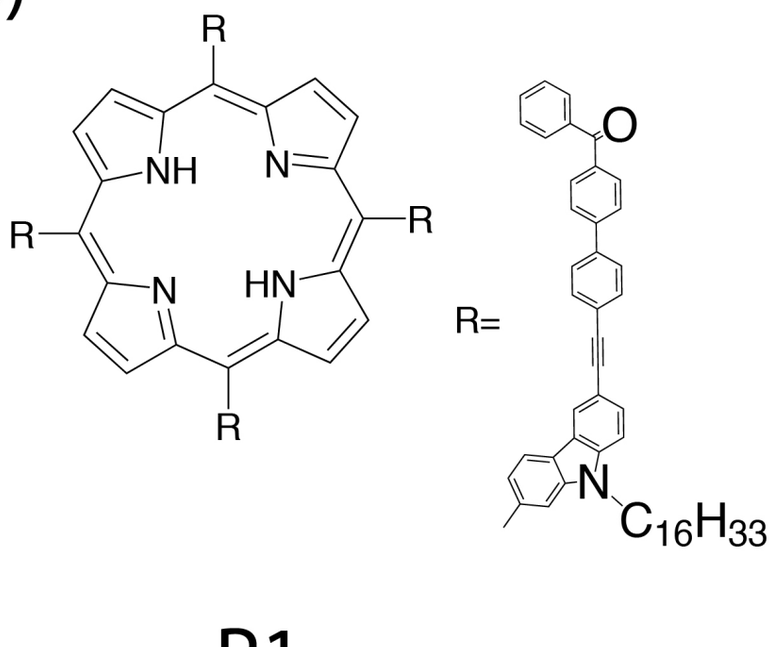
Zhang, C., Wang, Q., Long, H., & Zhang, W. (2011).
A Highly C_{70} Selective Shape-Persistent Rectangular Prism Constructed through One-Step Alkyne Metathesis.
Journal of the American Chemical Society, 133(51), 20995–21001.

a)



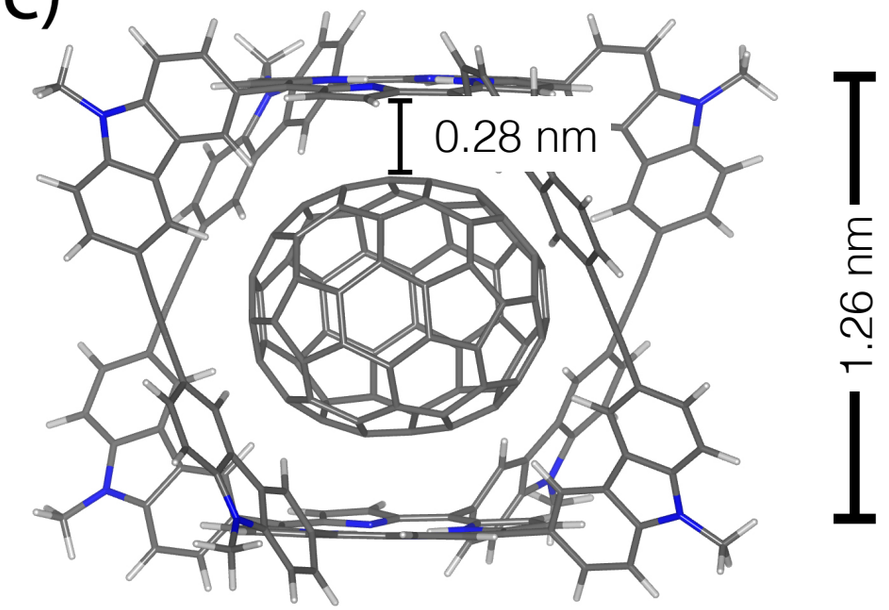
COP-5

b)



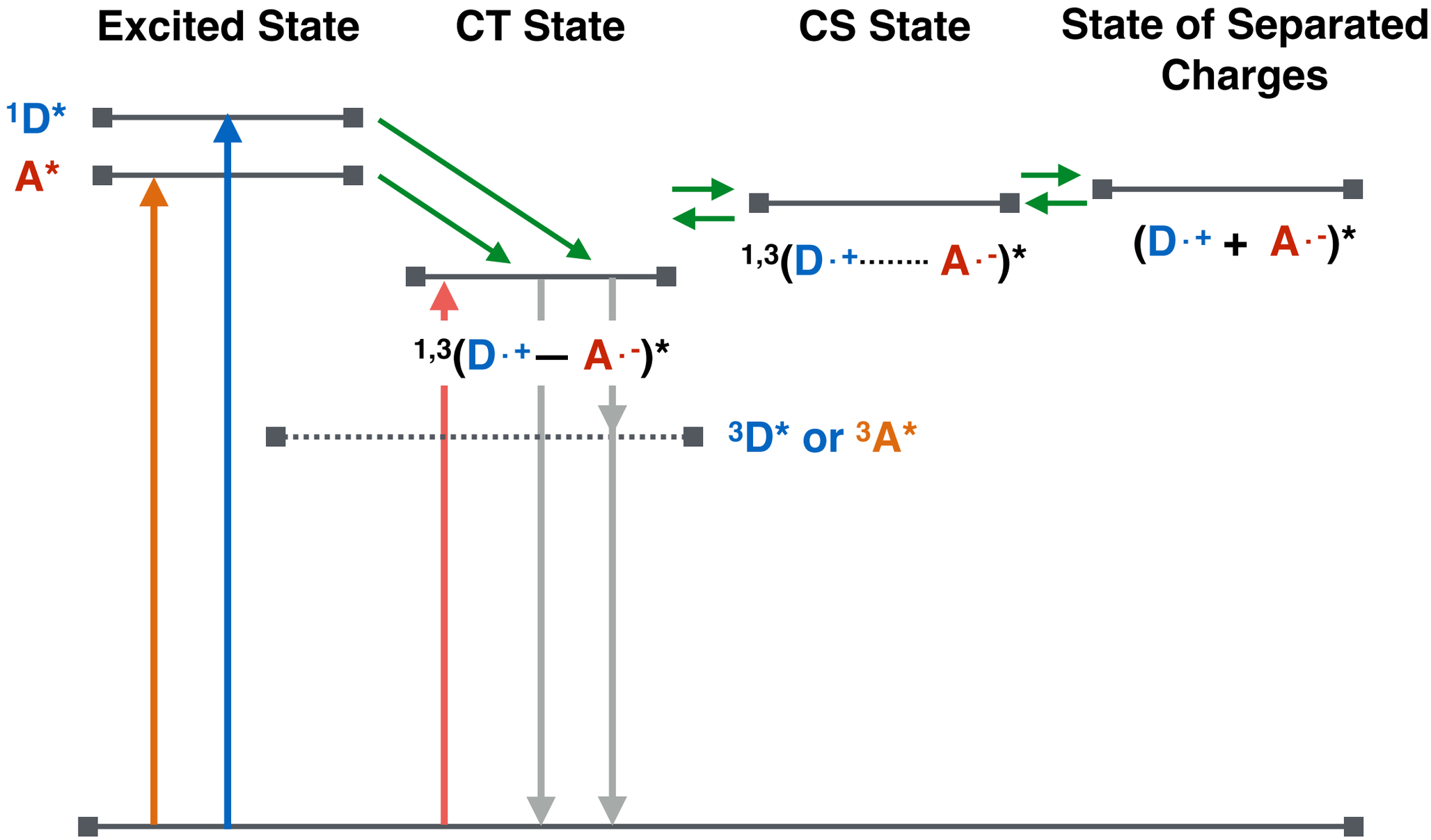
P1

c)



C_{70}@COP-5

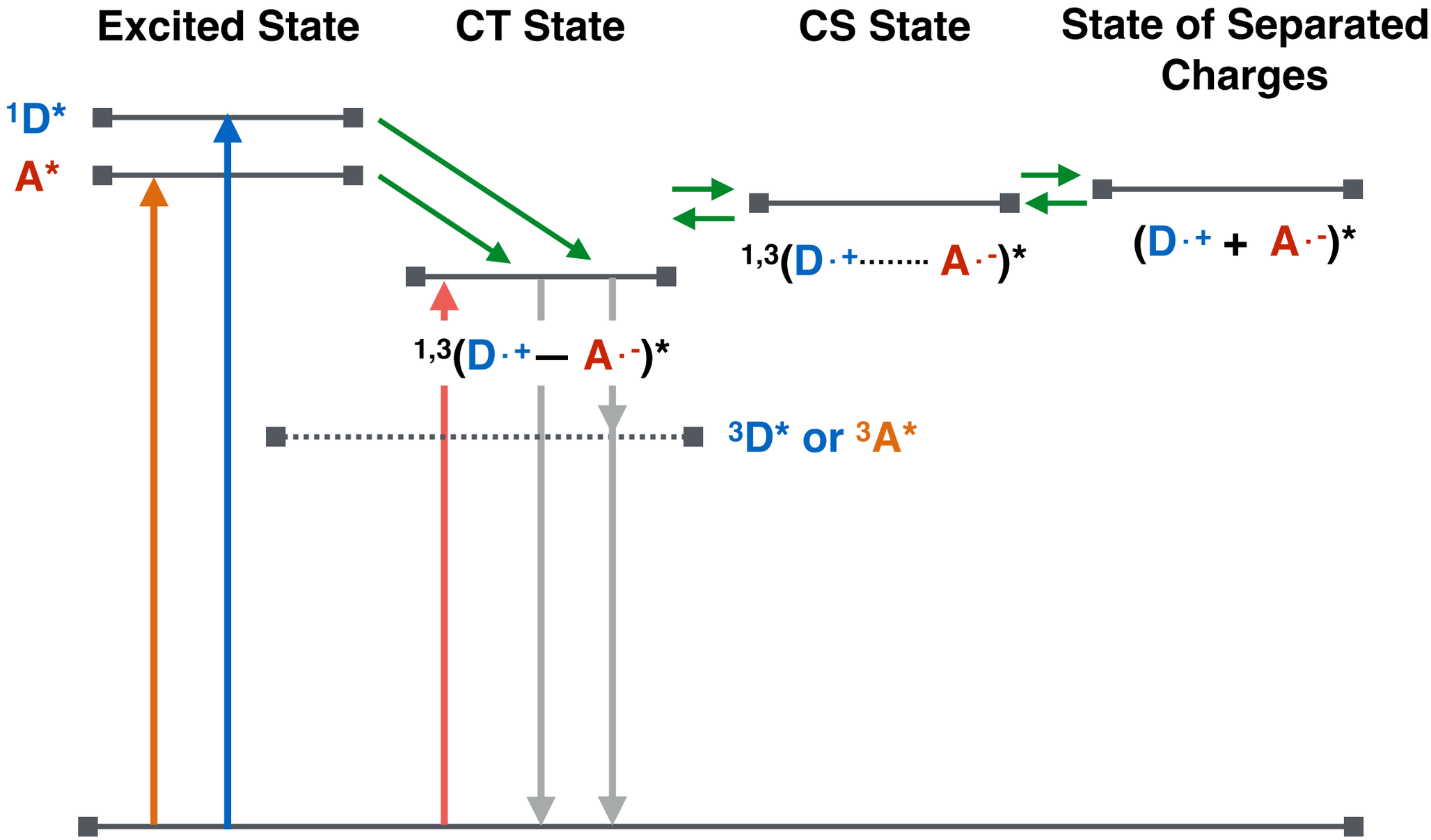
ΔG_{CS} in toluene = -0.27 eV; ΔG_{CS} in Benzonitrile = -0.95 eV



$$\Delta_{ET}G^{o} = N_A\left\{e\left[E^{o}\left(D^{+\bullet}/D\right)-E^{o}\left(A/A^{-\bullet}\right)\right]+\frac{z\left(D^{+\bullet}\right)z\left(A^{-\bullet}\right)e^{2}}{4\pi\varepsilon_0\varepsilon_r a}\right\}-\Delta E_{0,0}$$

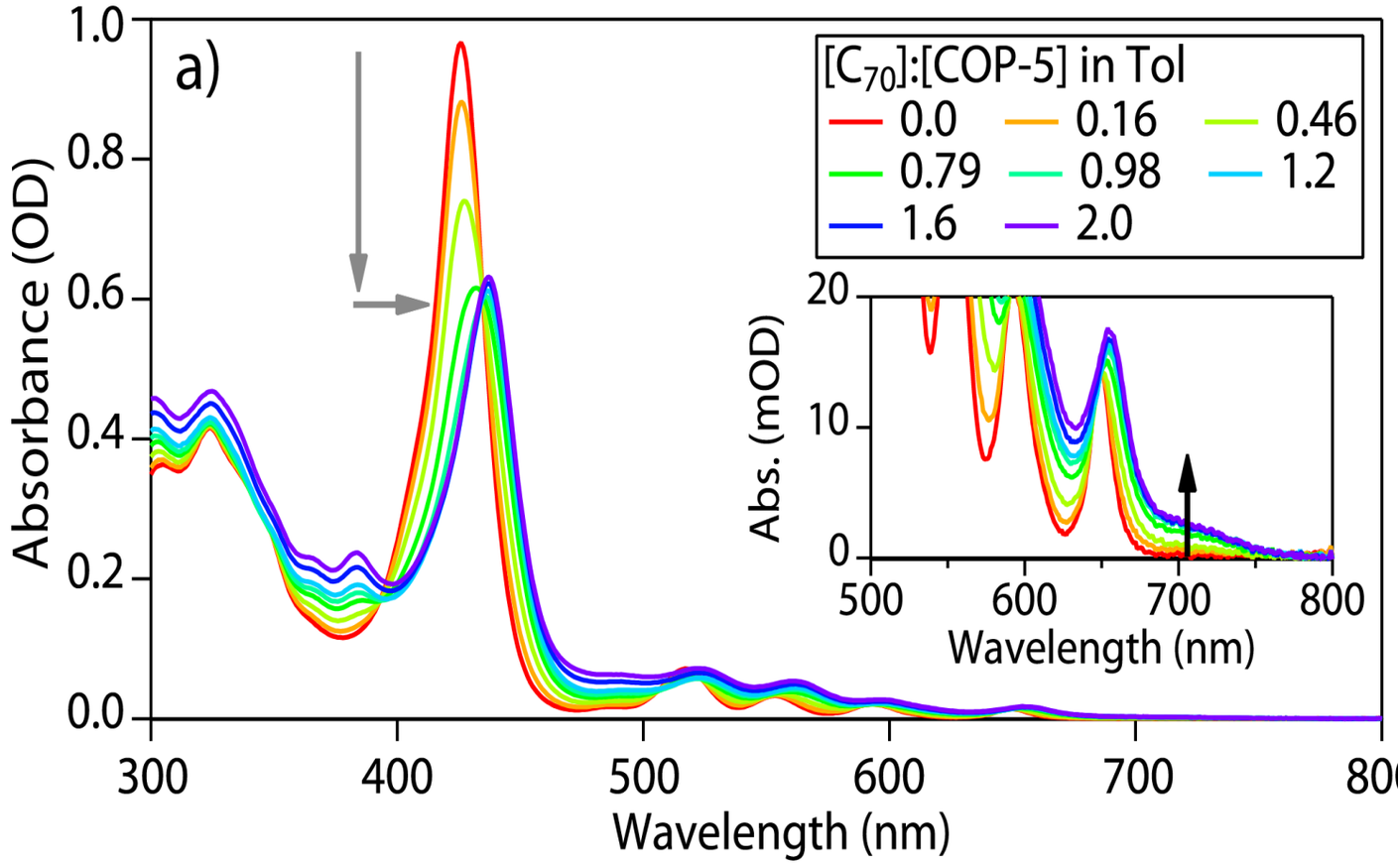
$$\Delta_{ET}G^{o} = \quad IP_D \quad - \quad EA_A \quad - \quad \frac{e^2}{4\pi\varepsilon_0\varepsilon_r a} \quad - E_{Exciton}$$

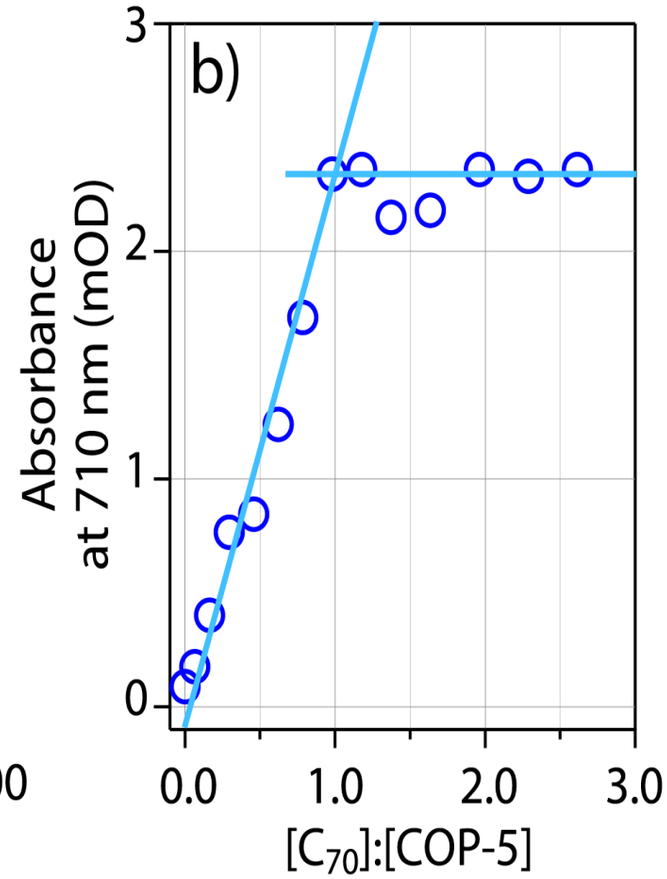
$$\Delta G_{CS} = \left(IP_D - E_{Exciton}\right) - EA_A = LUMO_D^{opt} - LUMO_A^{elec}$$

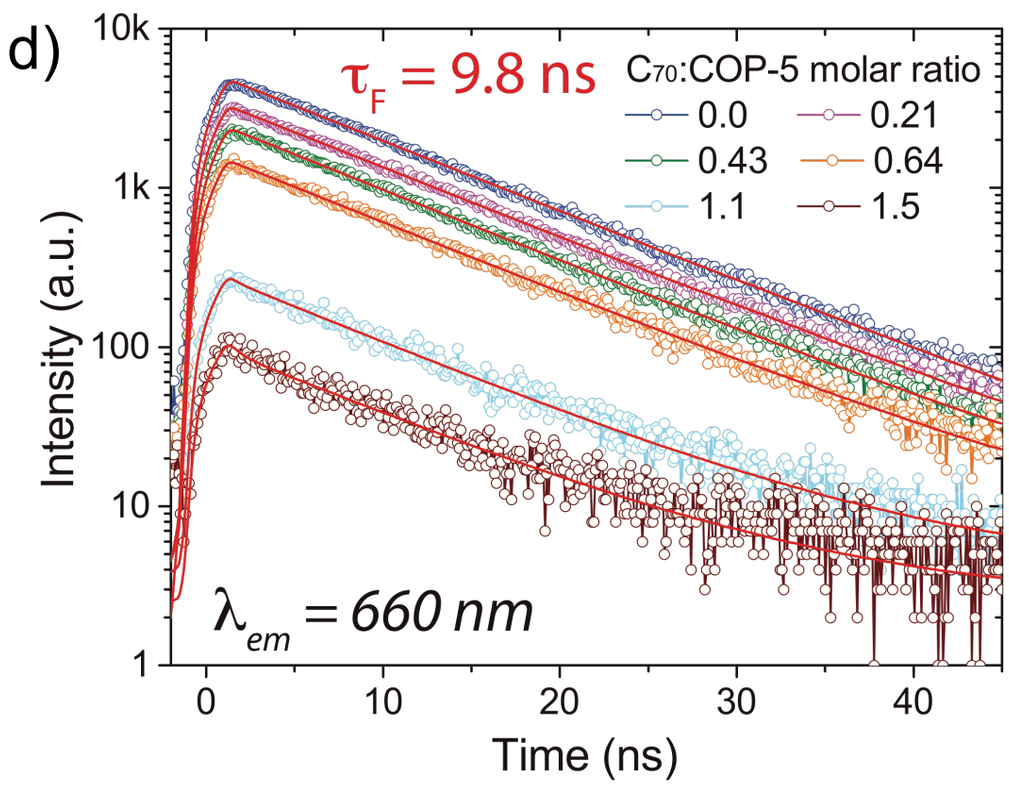


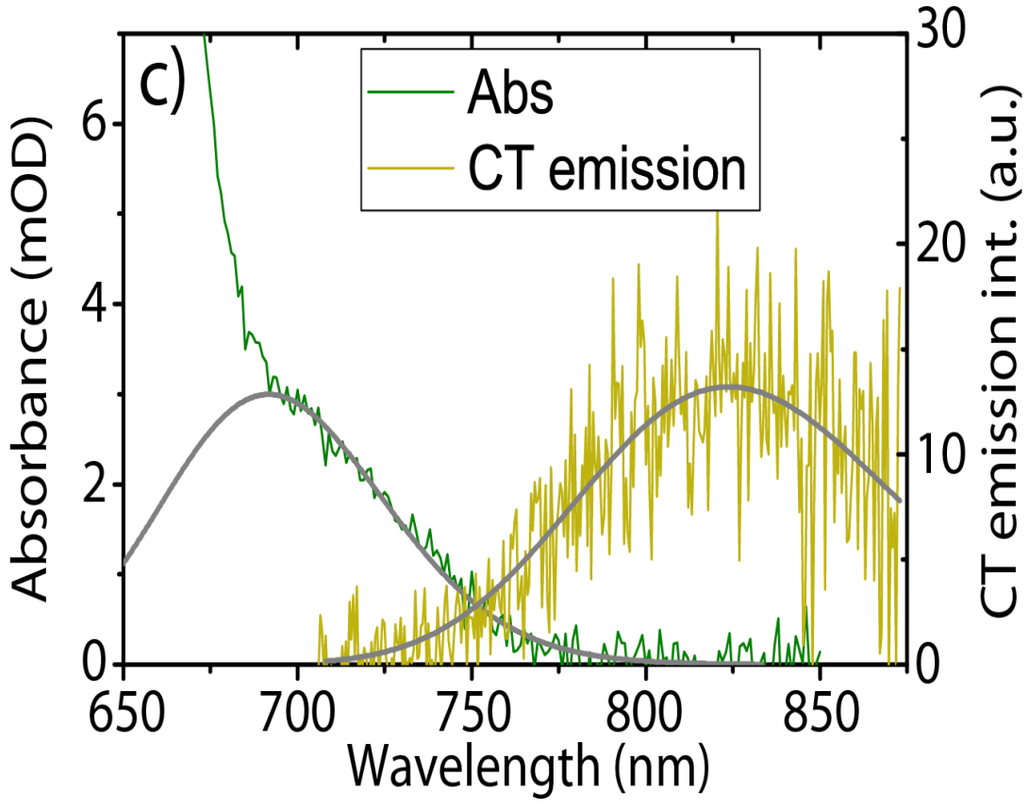
$$\Delta_{ET}G^{o} = N_{A}\left\{e\left[E^{o}\left(D^{+\bullet}/D\right) - E^{o}\left(A/A^{-\bullet}\right)\right] - \Delta E_{0,0} + \frac{z\left(D^{+\bullet}\right)z\left(A^{-\bullet}\right)e^{2}}{4\pi\varepsilon_{0}\varepsilon_{r}r_{DA}} - \frac{z\left(D^{+\bullet}\right)z\left(A^{-\bullet}\right)e^{2}}{4\pi\varepsilon_{0}}\left(\frac{1}{2r_{D}} + \frac{1}{2r_{A}}\right)\left(\frac{1}{\varepsilon_{EC}} - \frac{1}{\varepsilon_{S}}\right)\right\}$$

1:1 Complex and Static Quenching

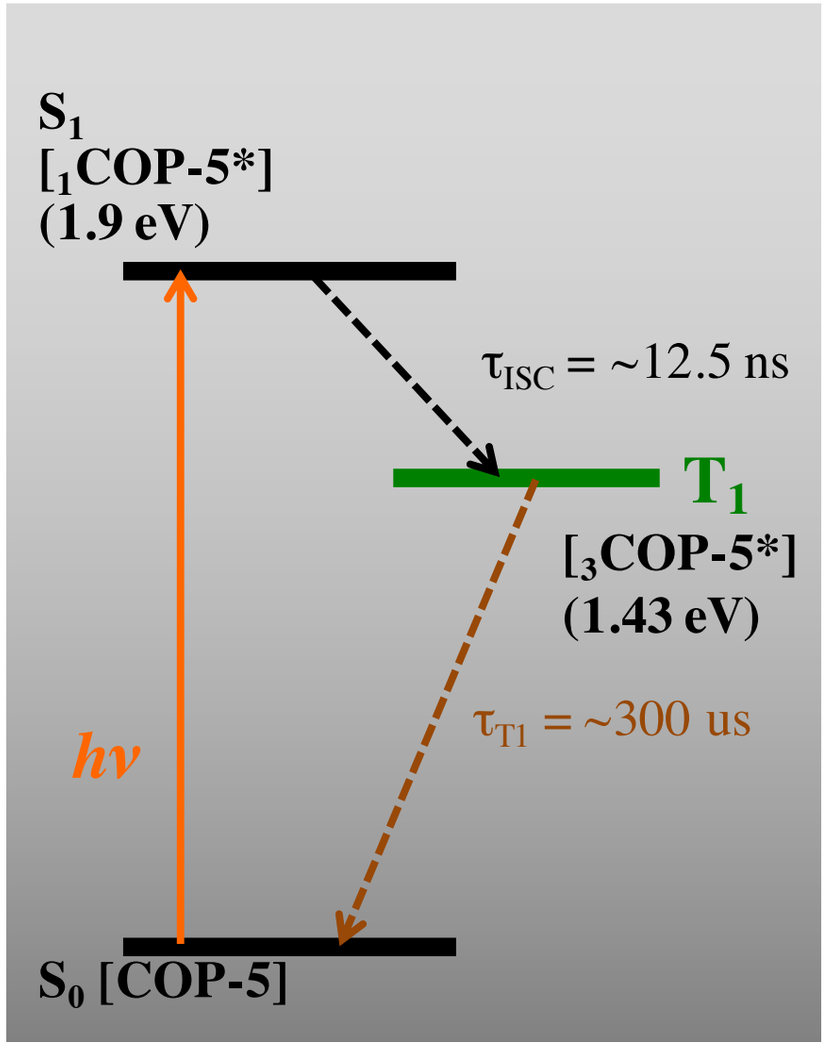


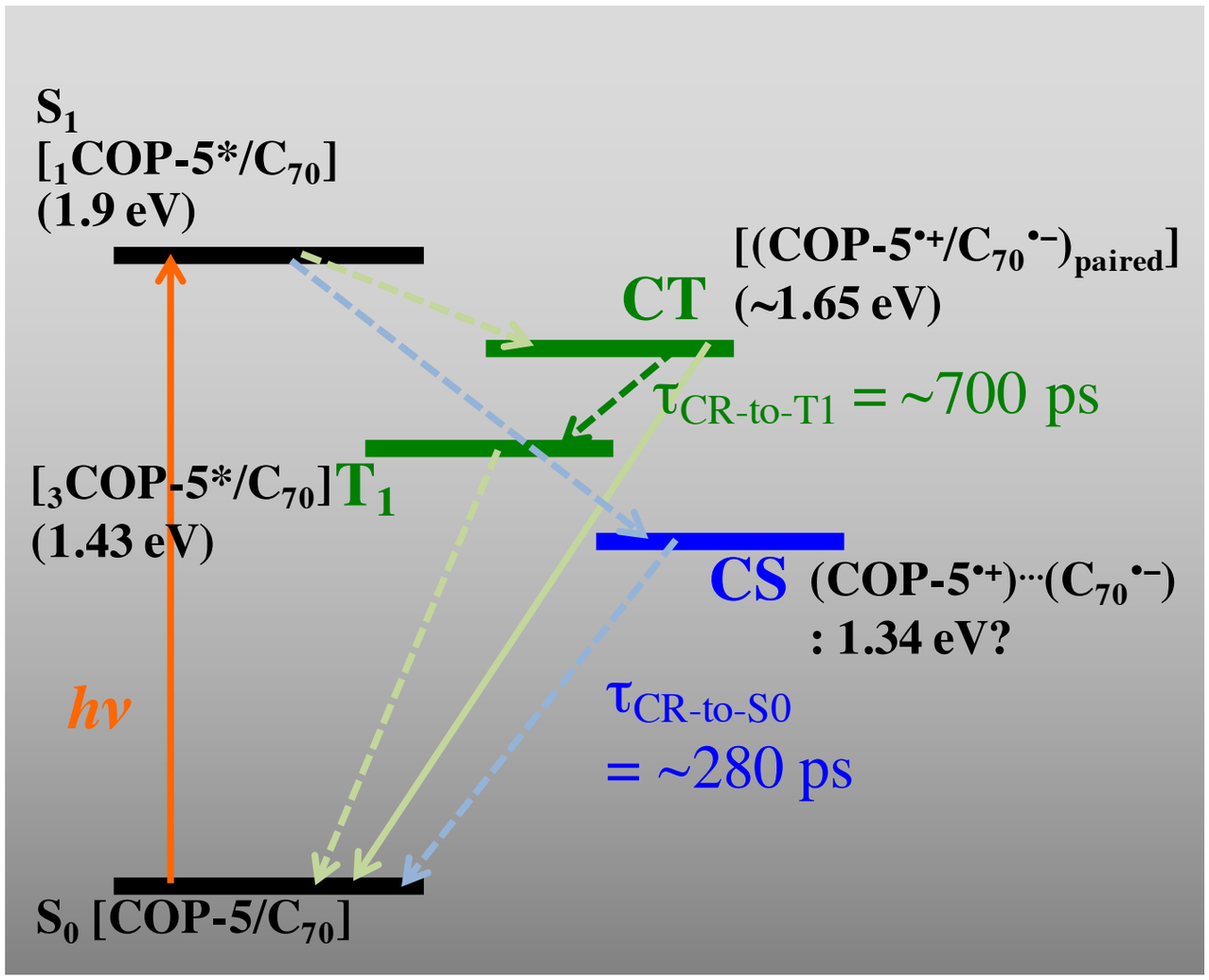


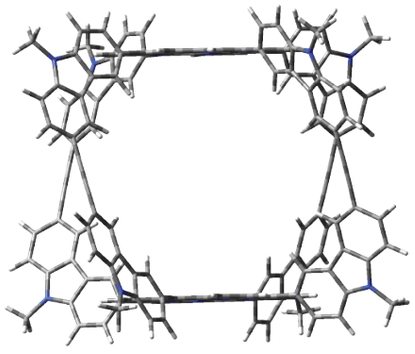


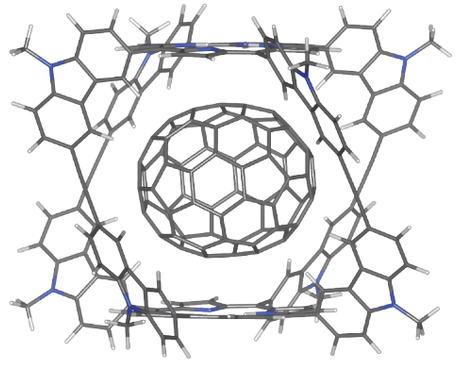


Photophysics summary









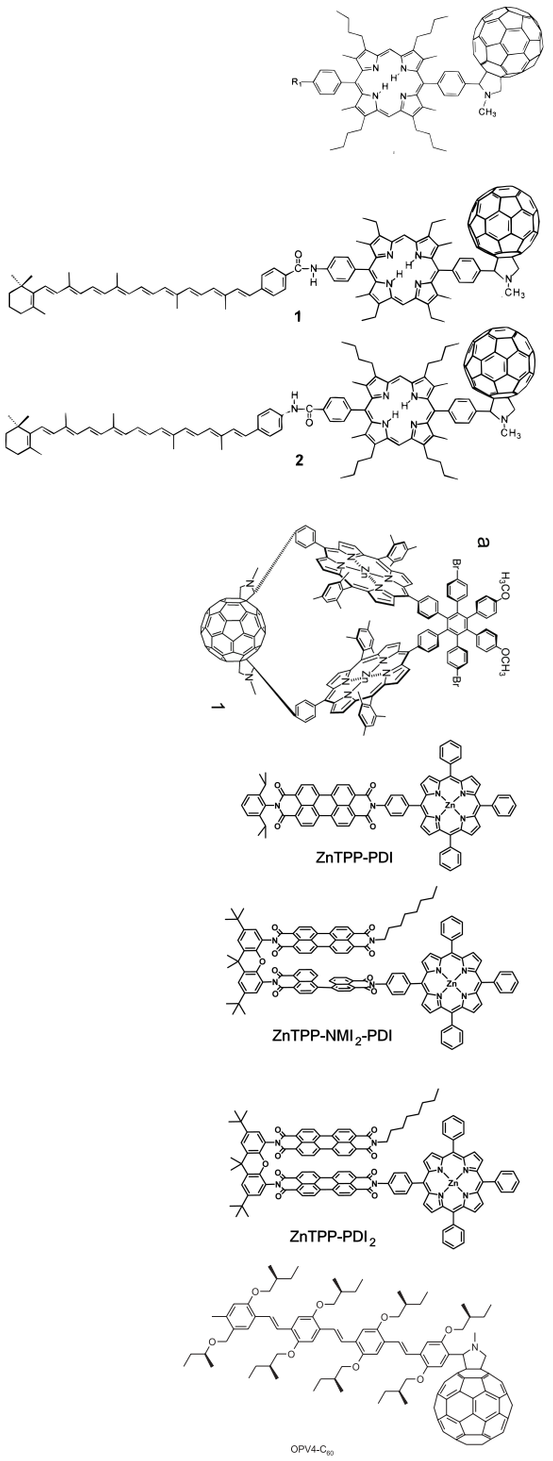
Long-lived charge-transfer state of a C_{70}-encapsulated bisporphyrin covalent organic polyhedron in a low dielectric medium.

Michael Ortiz, Sung Cho, Jens Niklas, Seonah Kim, Oleg G. Poluektov, Wei Zhang, Garry Rumbles, Jaehong Park

J. Am. Chem. Soc. 2017, 139, 4286–4289

Separation or recombination time /seconds

10^{-13} 10^{-12} 10^{-11} 10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6}

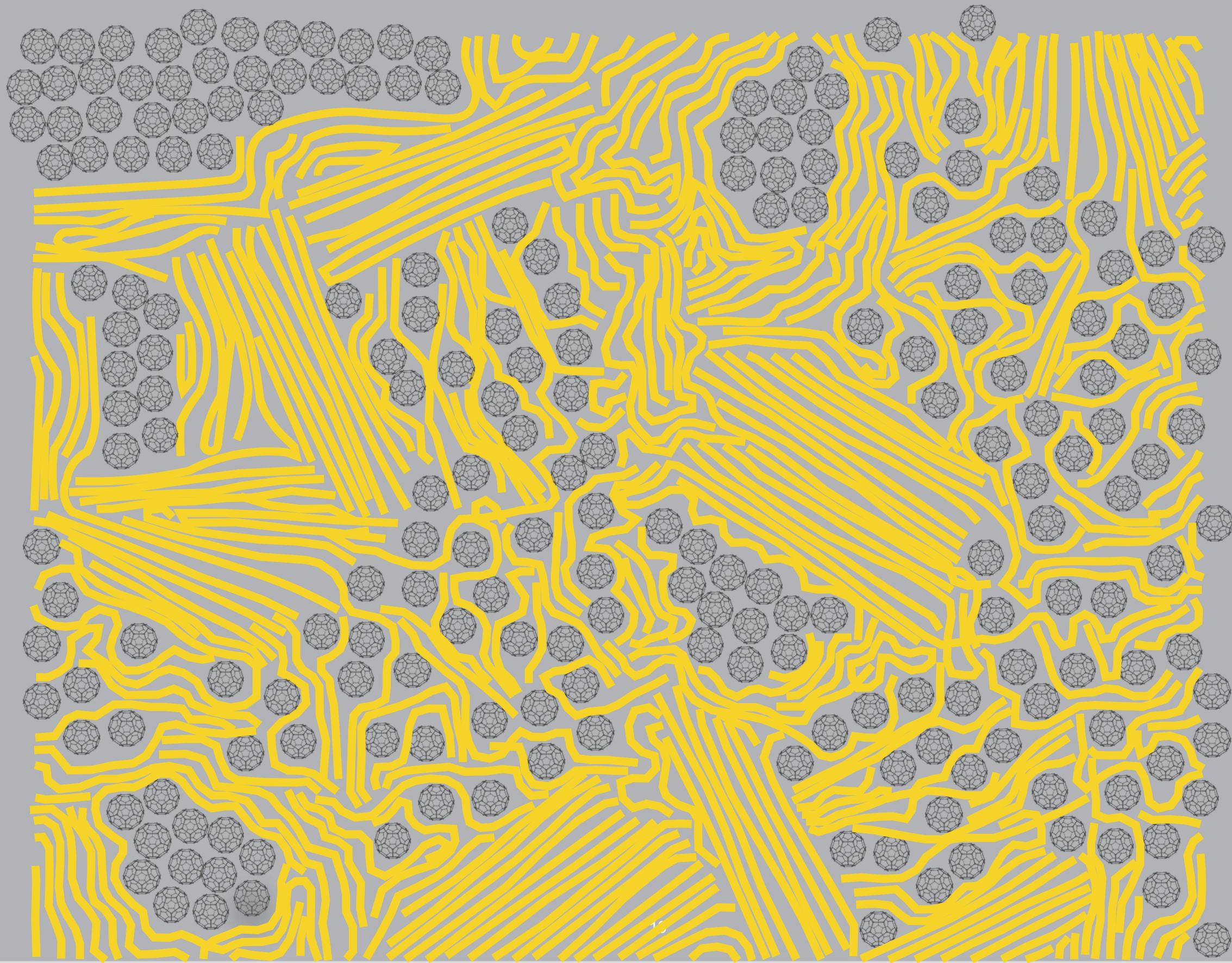


2%PCBM + RR-p3HT

0.0 0.2 0.4 0.6 0.8 1.0

Yield

A complex conjugated polymer:fullerene blend



Comments

- *Research cell efficiencies*
  - Notable exceptions
  - Device area
  - Certification
  - Nanostructured Materials for Type III Photovoltaics; Skabara, P., Malik, M. A., Eds.; The Royal Society of Chemistry, 2018; pp P001–P514.
- *Driving force for electron transfer and the relationship to V_{oc}*
  - Weller equation and Gibbs energy, not LUMO offset
  - Reorganiz(s)ation energy v ΔG
- *Charge-Transfer states, Charge-Separated states, and the state of separated charges*
  - CT states absorb and emit
  - CS states absorb very weakly, are generally associated with molecular triads and photosynthesis reaction center
  - State of separated charges are free of coulomb attraction, are extracted by devices and can b be readily detected using microwave conductivity
- *IP, E_A, v E_{ox}, E_{red}*
  - *Caution with connecting or combining these data*

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Application Window Opens	Application Window Closes*
March 1	July 1

Additional application windows to be determined.
*Applications submitted after the closing date will not be reviewed.

Candidates are selected based on eligibility, program expectations, and research proposals. Overriding consideration, when evaluating the application, will be the quality of the candidate. Successful candidates will serve a two-year term, with a possible third-year renewal paid with program funding (maximum three-year appointments). The Director's Fellowship includes a premium salary rate, additional funding for conferences/presentations, competitive benefits package, and relocation assistance (for moves greater than 50 miles from NREL).