King Abdullah University of Science and Technology

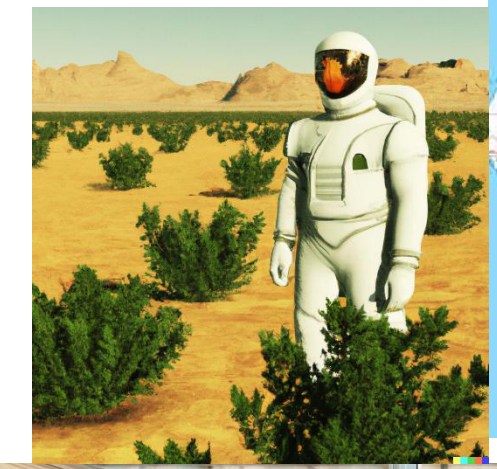
Organic Semiconductor Devices: from energetics to green processing

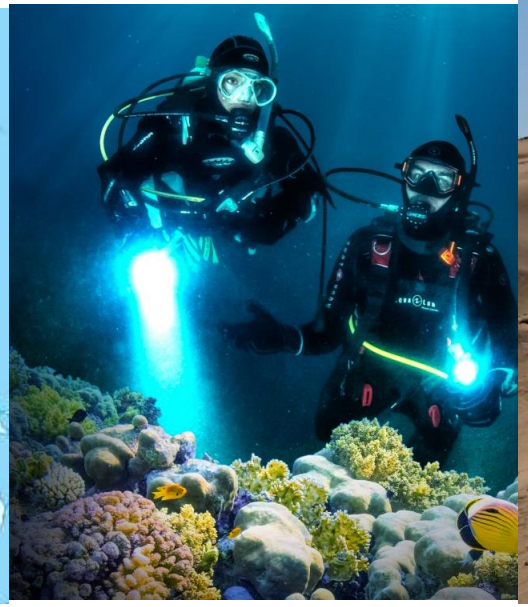
Derya Baran

Associate Professor of Materials Science and Engineering Program, KAUST

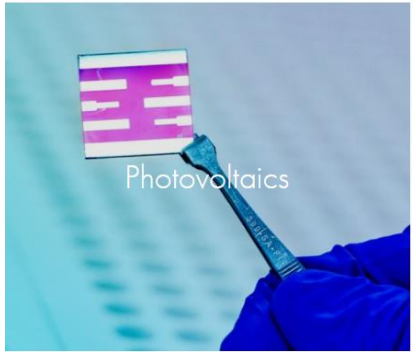
Sino-German Workshop ERLANGEN 2024

KAUST/ OMEGALAB

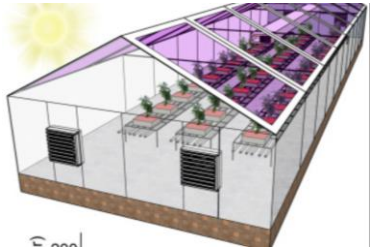


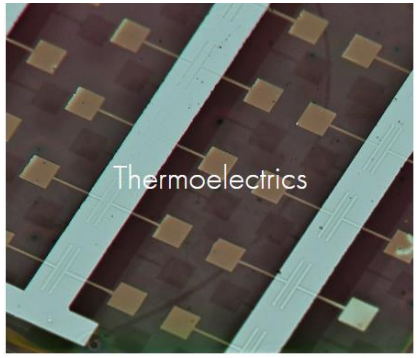


DERYA BARAN
ORGANIC/HYBRID MATERIALS FOR ENERGY APPLICATIONS(www.omegalabresearch.com)

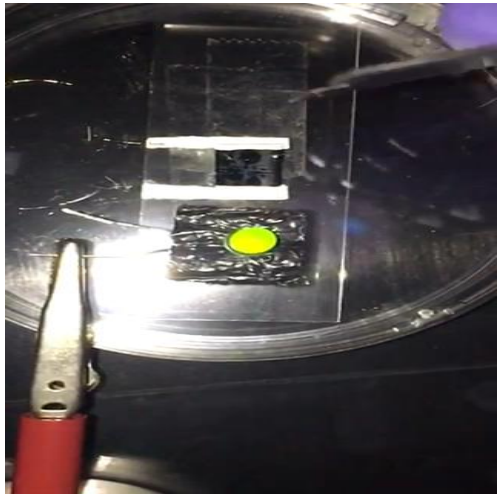


Solution processed PV
Stability and reliability of PV

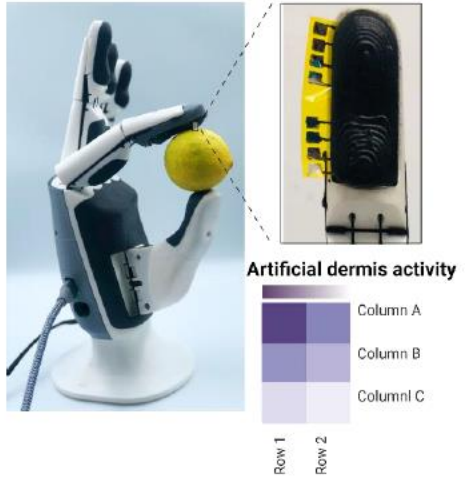




Thermoelectrics
Charge transport in n-type
Stretchable healable TE



Printing,3D printing, Micro printing
Conductive composites
Electronic Skin



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King Abdullah University of Science and Technology

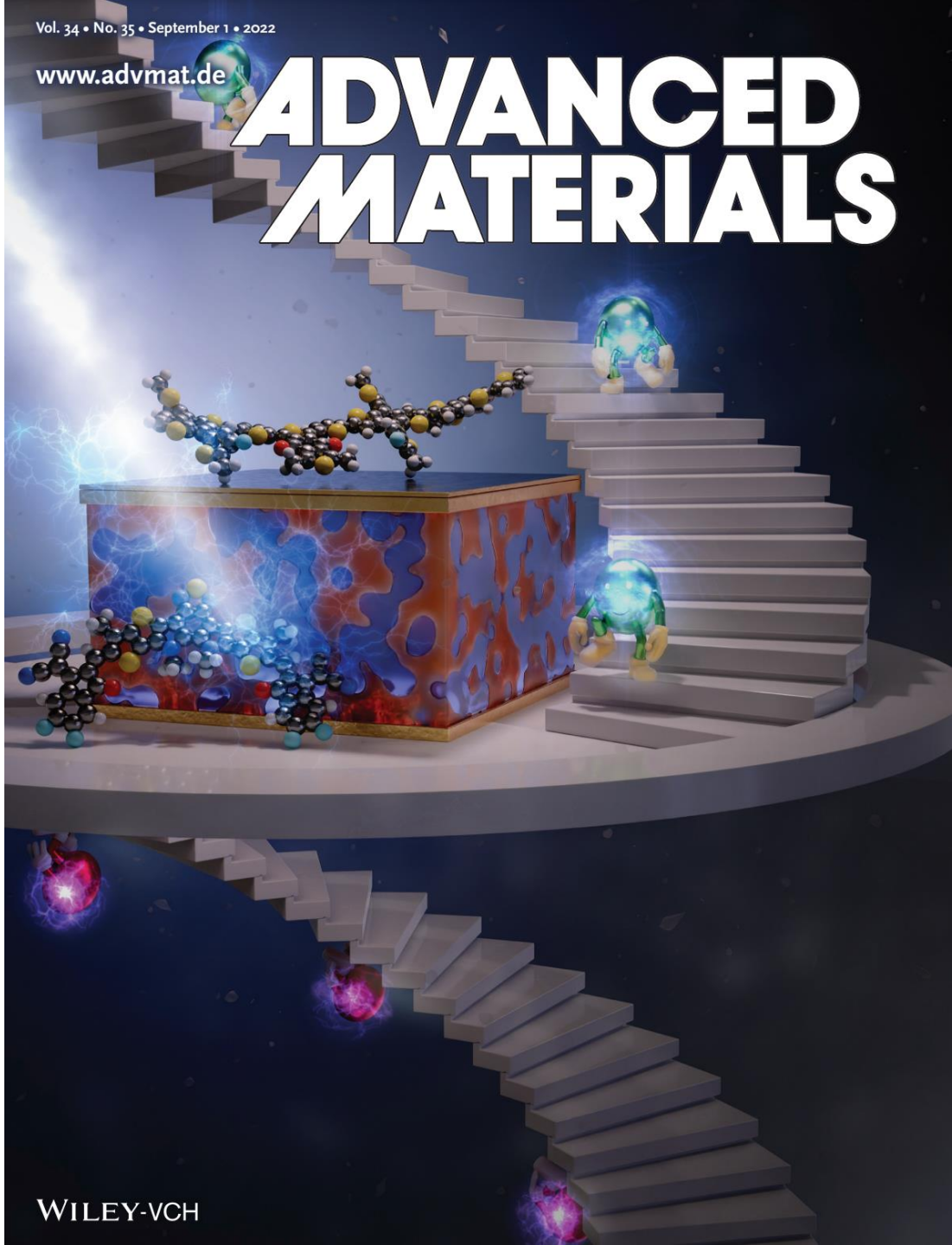
KAUST SOLAR CENTER

Energy level determination of organic semiconductors for solar cells

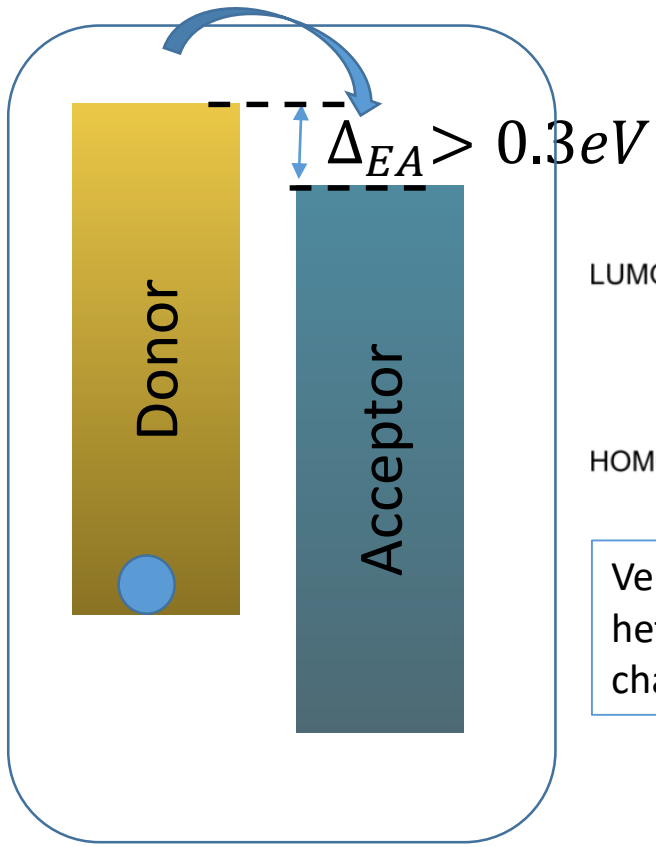
Anirudh Sharma

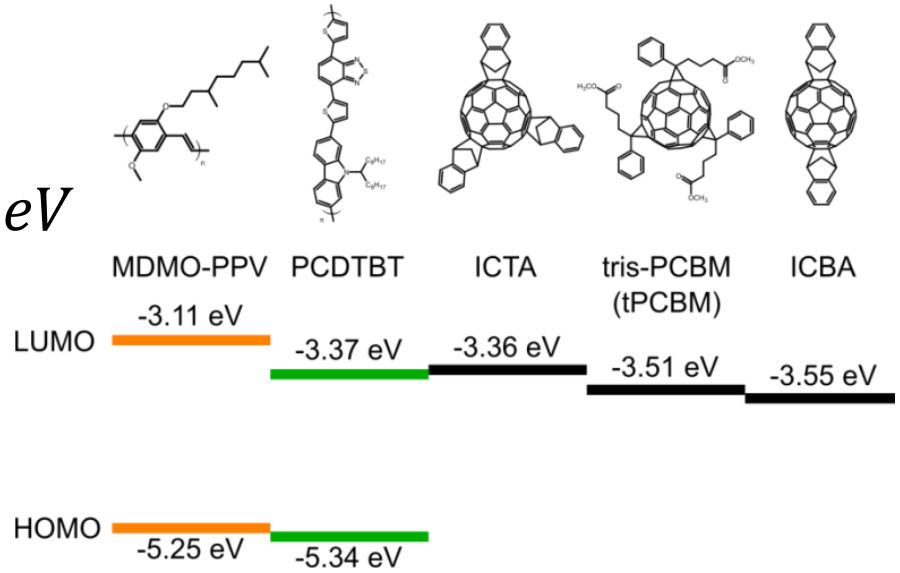
Jules Bertrandie

Adv. Mater. 2022, 34, 2202575.



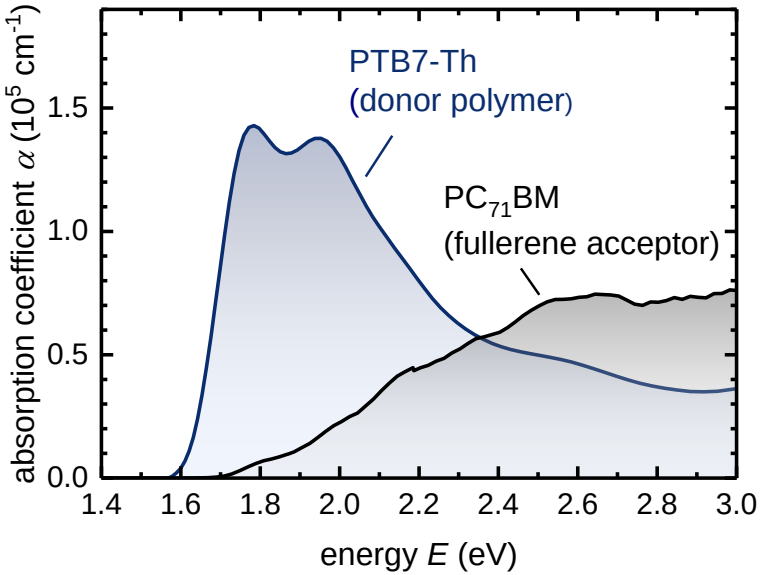
Why energetics matter?



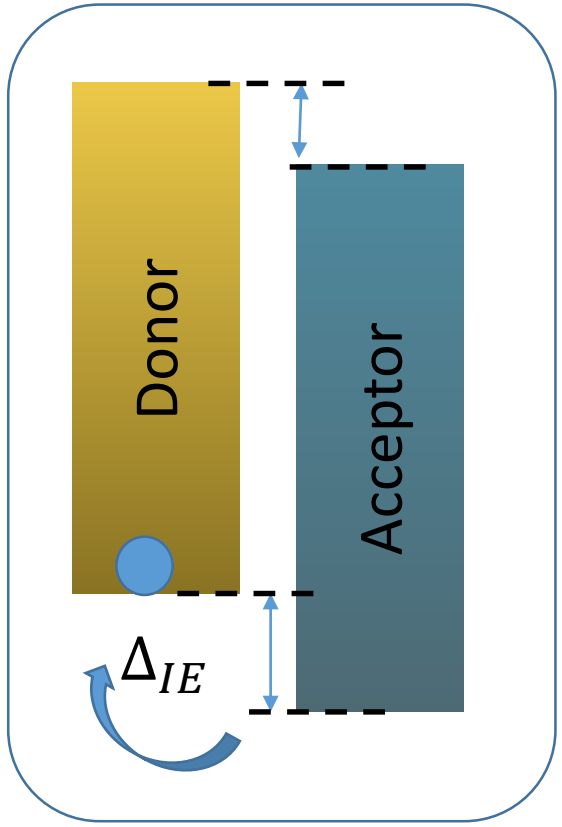


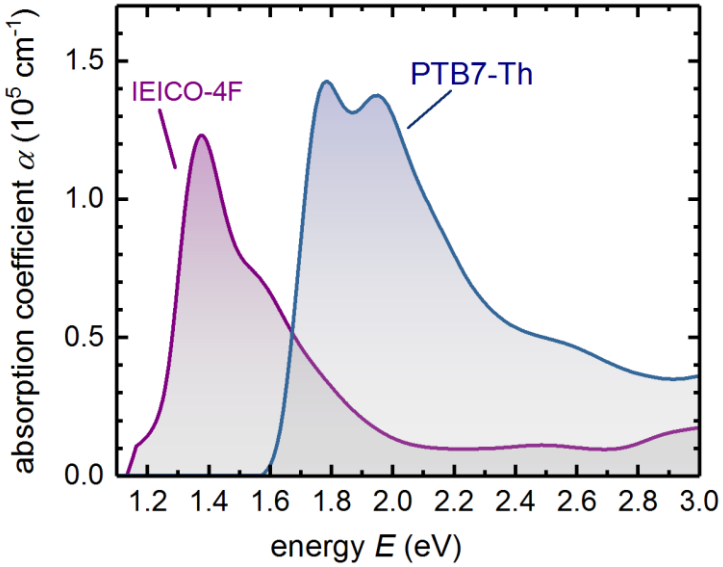
Very little driving energy is required at the heterojunction to dissociate excitons and generate free charges

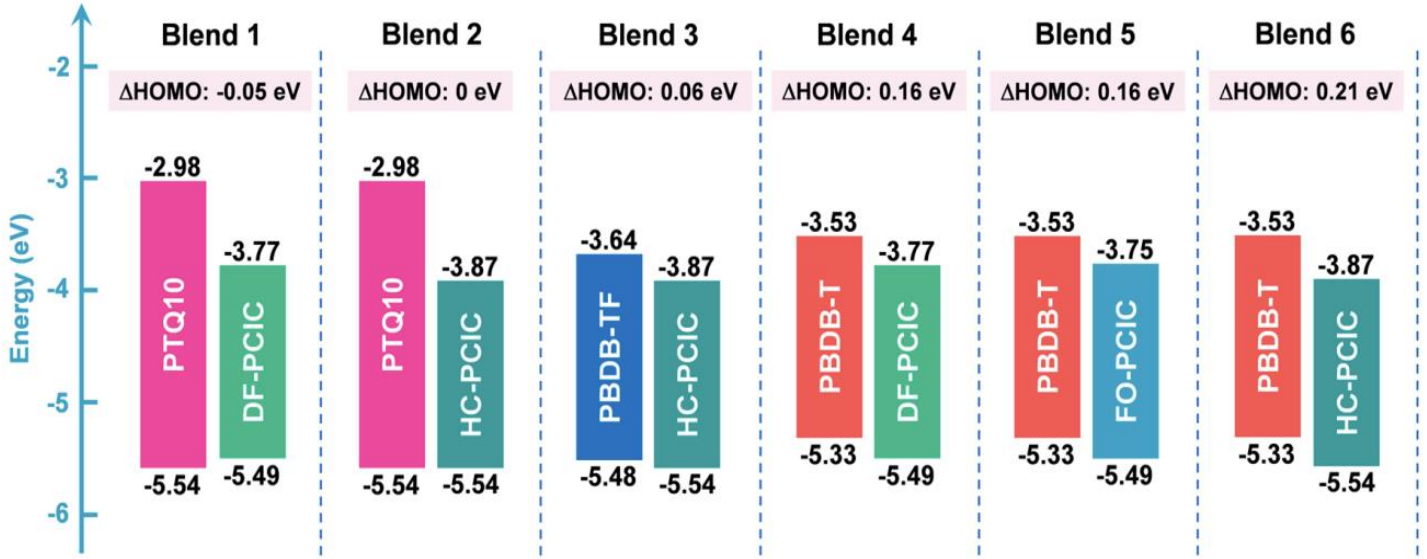
Fullerenes mostly had wider bandgap than donors



Why energetics matter?

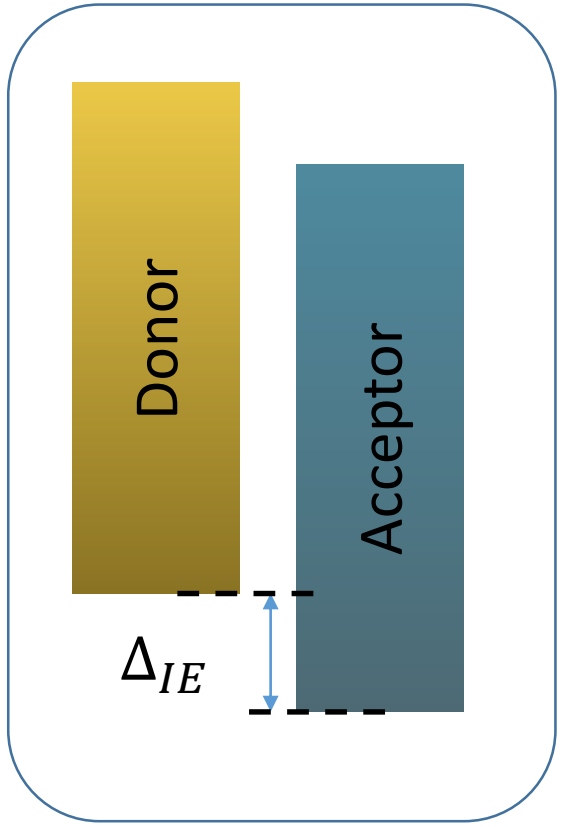






S. LI, *J. Am. Chem. Soc.* 2019, 141, 7, 3073–3082

Offset or no offset?

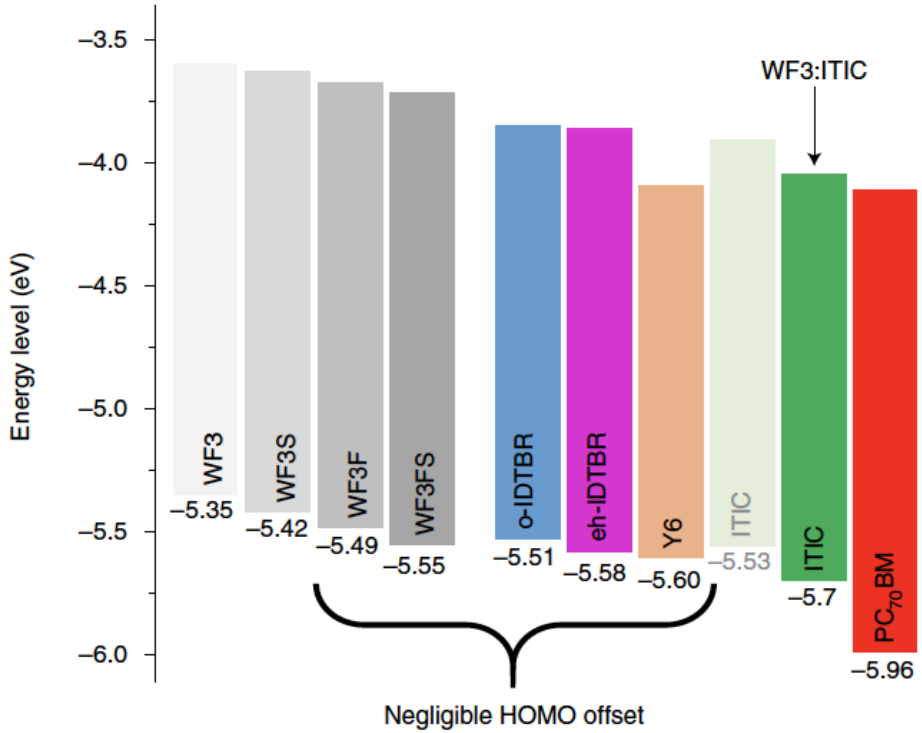


nature energy
ARTICLES
https://doi.org/10.1038/s41560-020-00684-7
Check for updates

The role of exciton lifetime for charge generation in organic solar cells at negligible energy-level offsets

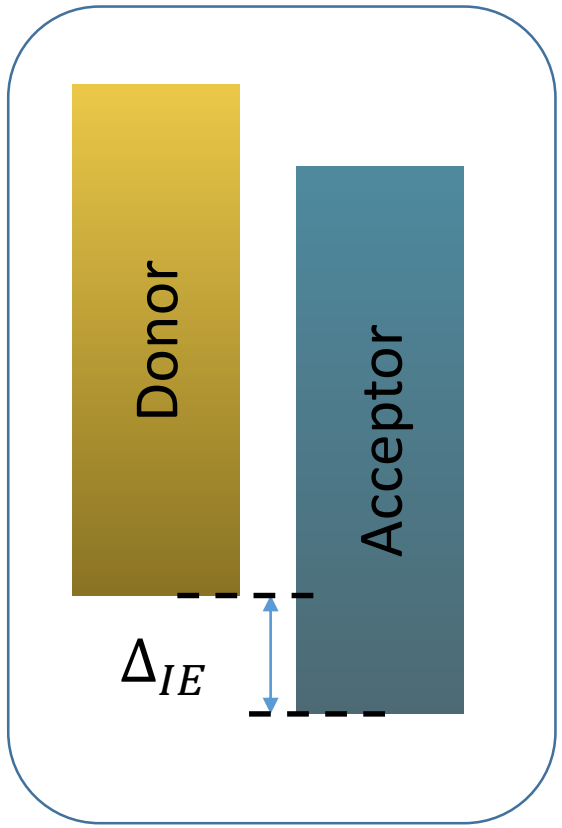
Andrej Classen[1], Christos L. Chochos[2,3], Larry Lüer[1]✉, Vasilis G. Gregoriou[2,4], Jonas Wortmann[1], Andres Osvet[1], Karen Forberich[1], Iain McCulloch[5,6], Thomas Heumüller[1,7]✉ and Christoph J. Brabec[1,7,8]✉

Organic solar cells utilize an energy-level offset to generate free charge carriers. Although a very small energy-level offset increases the open-circuit voltage, it remains unclear how exactly charge generation is affected. Here we investigate organic solar cell blends with highest occupied molecular orbital energy-level offsets (ΔE_{HOMO}) between the donor and acceptor that range from 0 to 300 meV. We demonstrate that exciton quenching at a negligible ΔE_{HOMO} takes place on timescales that approach the exciton lifetime of the pristine materials, which drastically limits the external quantum efficiency. We quantitatively describe this finding via the Boltzmann stationary-state equilibrium between charge-transfer states and excitons and further reveal a long exciton lifetime to be decisive in maintaining an efficient charge generation at a negligible ΔE_{HOMO}. Moreover, the Boltzmann equilibrium quantitatively describes the major reduction in non-radiative voltage losses at a very small ΔE_{HOMO}. Ultimately, highly luminescent near-infrared emitters with very long exciton lifetimes are suggested to enable highly efficient organic solar cells.



Classen, et al., Nature Energy, 2020, 10.1038/s41560-020-00684-7

Offset or no offset?

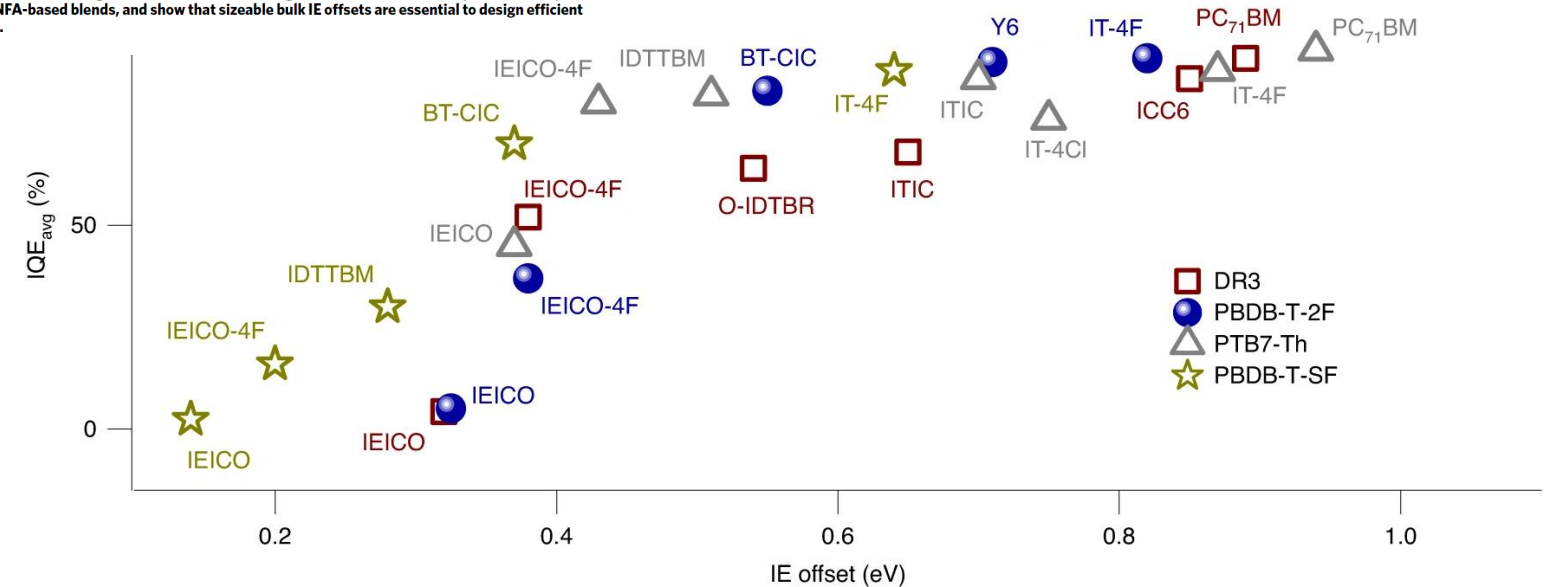


ARTICLES
https://doi.org/10.1038/s41563-020-00835-x
nature materials

Intrinsic efficiency limits in low-bandgap non-fullerene acceptor organic solar cells

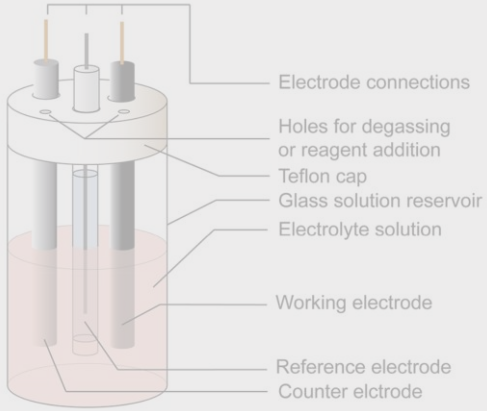
Safakath Karuthedath[1,5], Julien Gorenflot[1,5], Yuliar Firdaus[1], Neha Chaturvedi[1], Catherine S. P. De Castro[1,5], George T. Harrison[1], Jafar I. Khan[1], Anastasia Markina[2], Ahmed H. Balawi[1], Top Archie Dela Peña[1], Wenlan Liu[2], Ru-Ze Liang[1], Anirudh Sharma[1], Sri H. K. Paleti[1], Weimin Zhang[1], Yuanbao Lin[1], Erkki Alarousu[1], Dalaver H. Anjum[3], Pierre M. Beaujuge[1], Stefaan De Wolf[1], Iain McCulloch[1,4], Thomas D. Anthopoulos[1], Derya Baran[1], Denis Andrienko[2]✉ and Frédéric Laquai[1]✉

In bulk heterojunction (BHJ) organic solar cells (OSCs) both the electron affinity (EA) and ionization energy (IE) offsets at the donor–acceptor interface should equally control exciton dissociation. Here, we demonstrate that in low-bandgap non-fullerene acceptor (NFA) BHJs ultrafast donor-to-acceptor energy transfer precedes hole transfer from the acceptor to the donor and thus renders the EA offset virtually unimportant. Moreover, sizeable bulk IE offsets of about 0.5 eV are needed for efficient charge transfer and high internal quantum efficiencies, since energy level bending at the donor–NFA interface caused by the acceptors' quadrupole moments prevents efficient exciton-to-charge-transfer state conversion at low IE offsets. The same bending, however, is the origin of the barrier-less charge transfer state to free charge conversion. Our results provide a comprehensive picture of the photophysics of NFA-based blends, and show that sizeable bulk IE offsets are essential to design efficient BHJ OSCs based on low-bandgap NFAs.

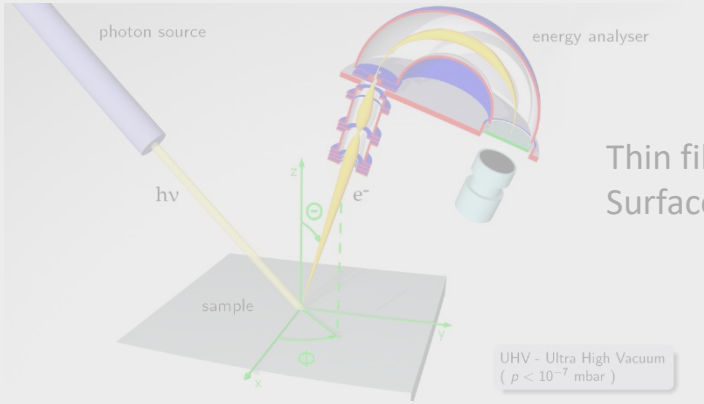


S. Karuthedath, *Nat. Mater.* **20**, 378–384 (2021)

Motivation



Solutions; thin films
Presence of electrolyte
Electrochemical instability
Lack of electrochemical reversibility



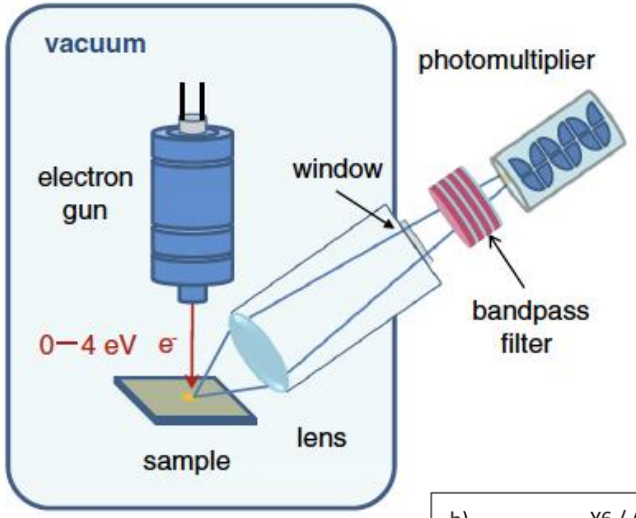
Thin films
Surface sensitive

Define a criteria for determining the energetics of OSCs

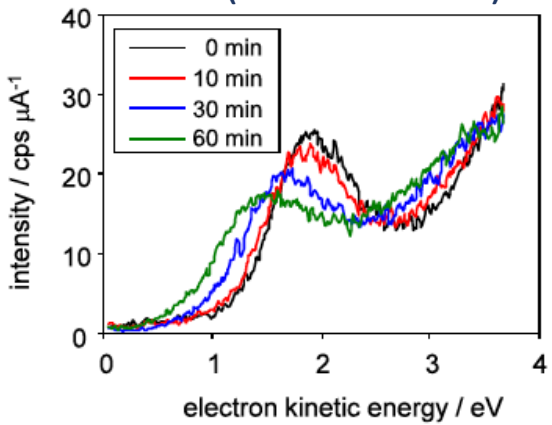
Correlation between material energetics – Voc

Establish material-property relationship for design rules

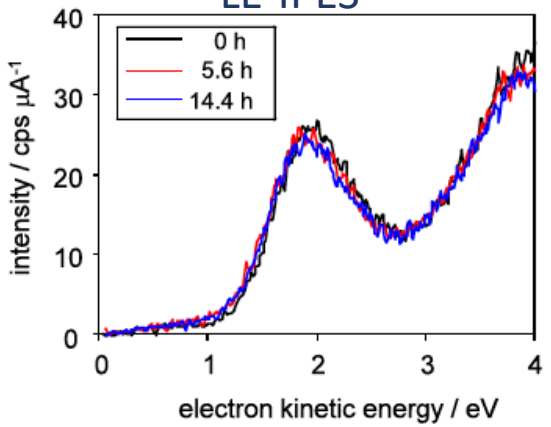
Method of measurements



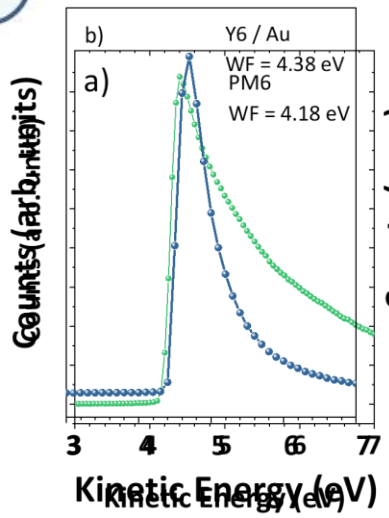
IPES (conventional)

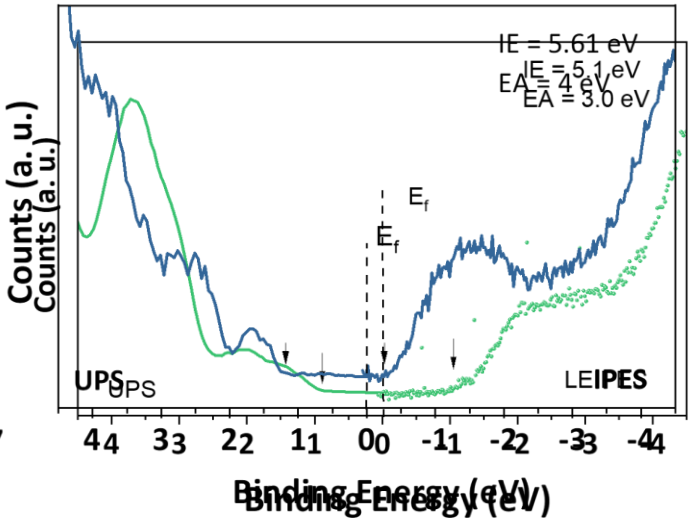


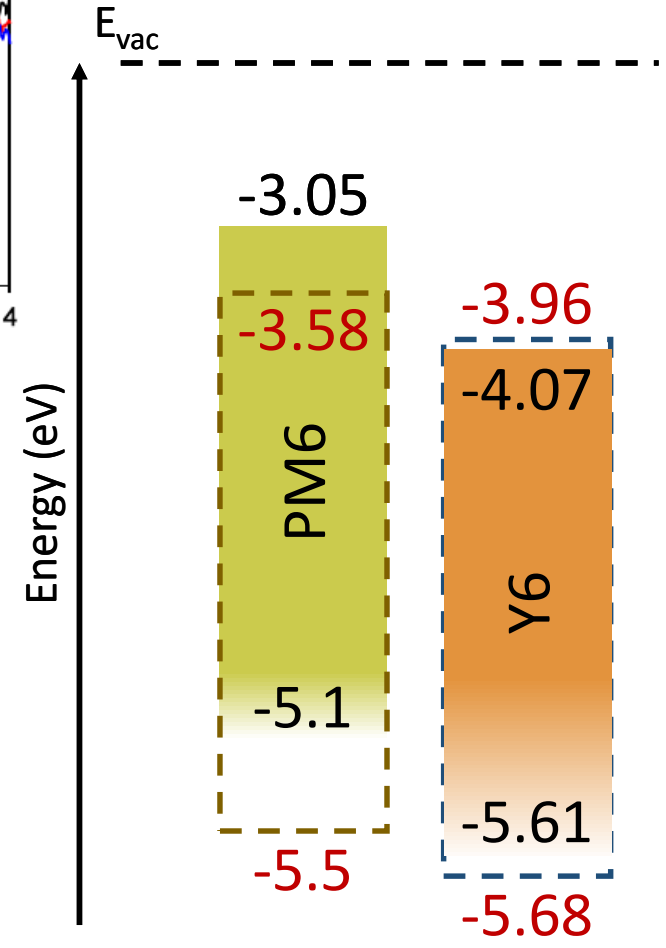
LE-IPES



PM6

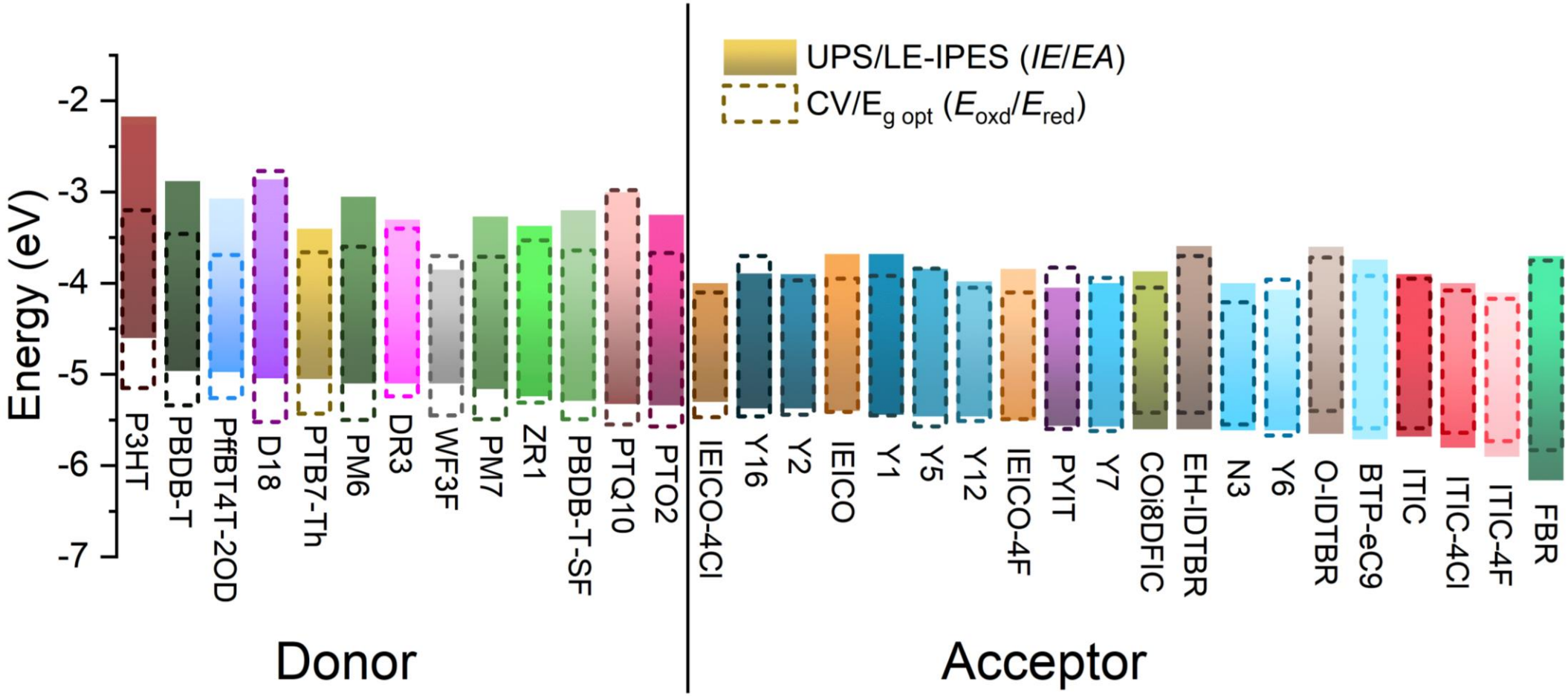






Yoshida, Jurnal of Physical Chemistry C, 2014, 118, 42
Yoshida, Chemical Physics Letters, 2012, 539, 180

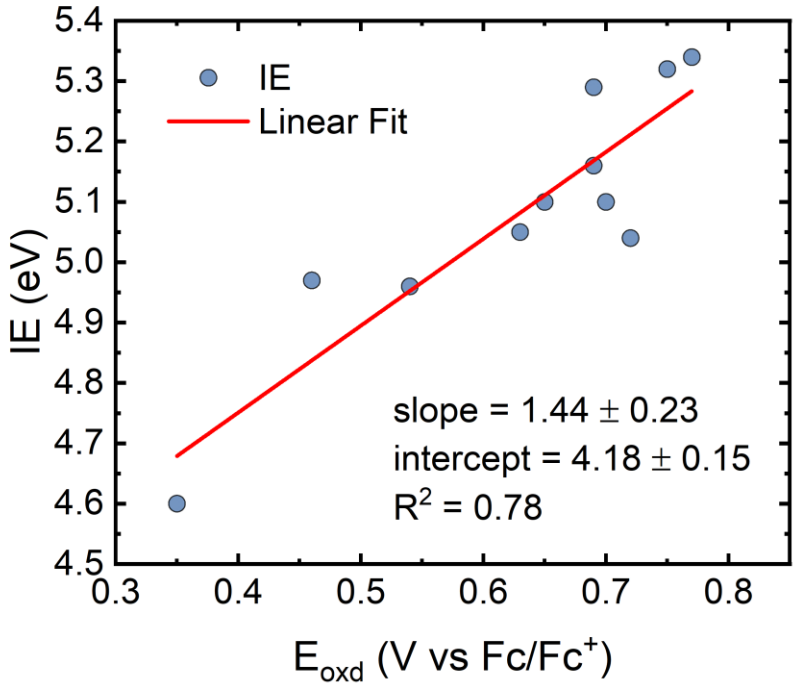
Library of Energetics

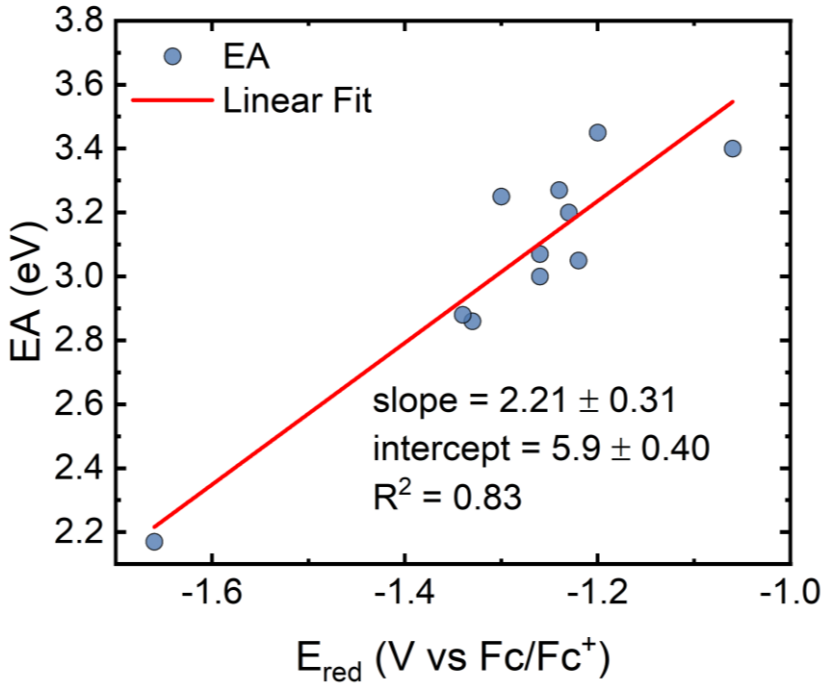


Bertrandie, et al., Advanced Materials, 2022, 4 (35), e2202575

Correlating Redox Potentials with IE/EA

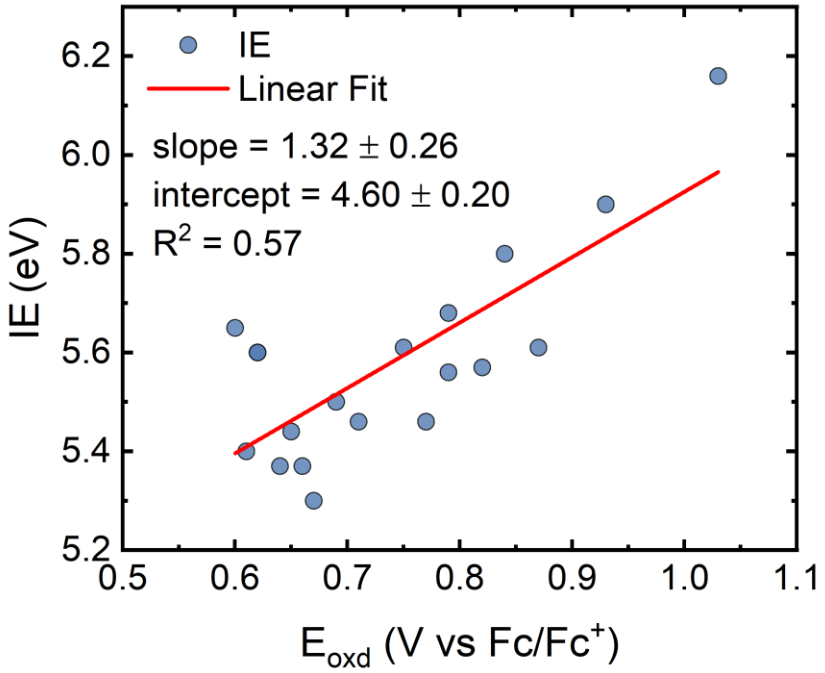
Donor Polymers

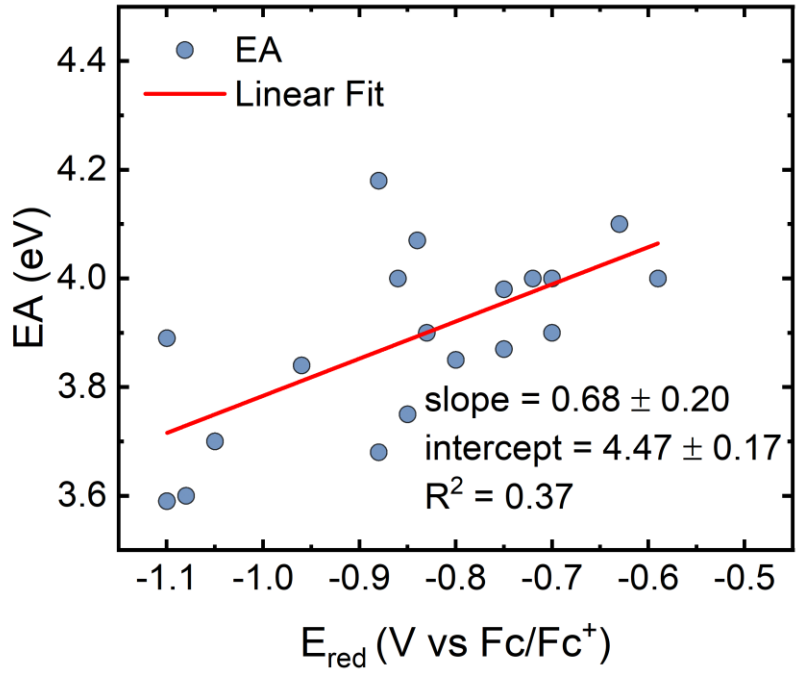




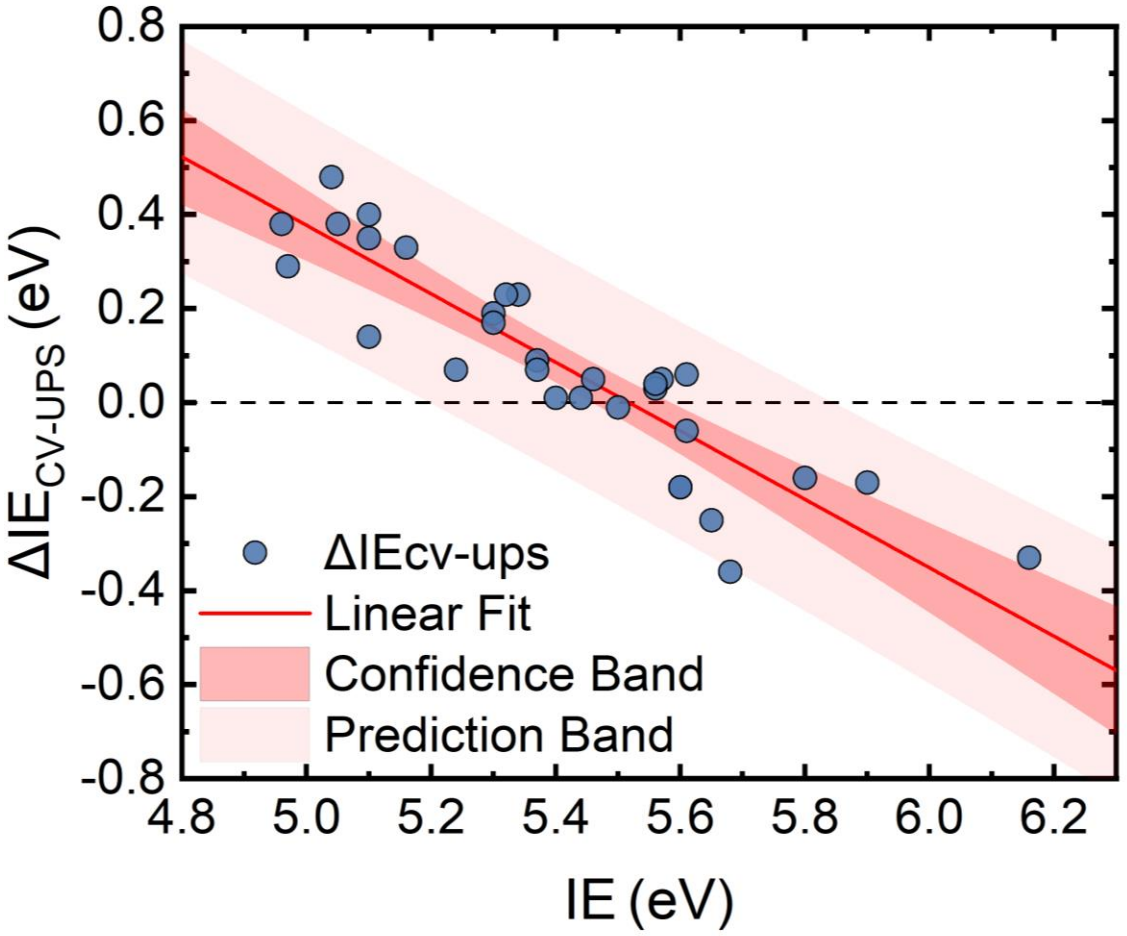
Correlating Redox Potentials with IE/EA

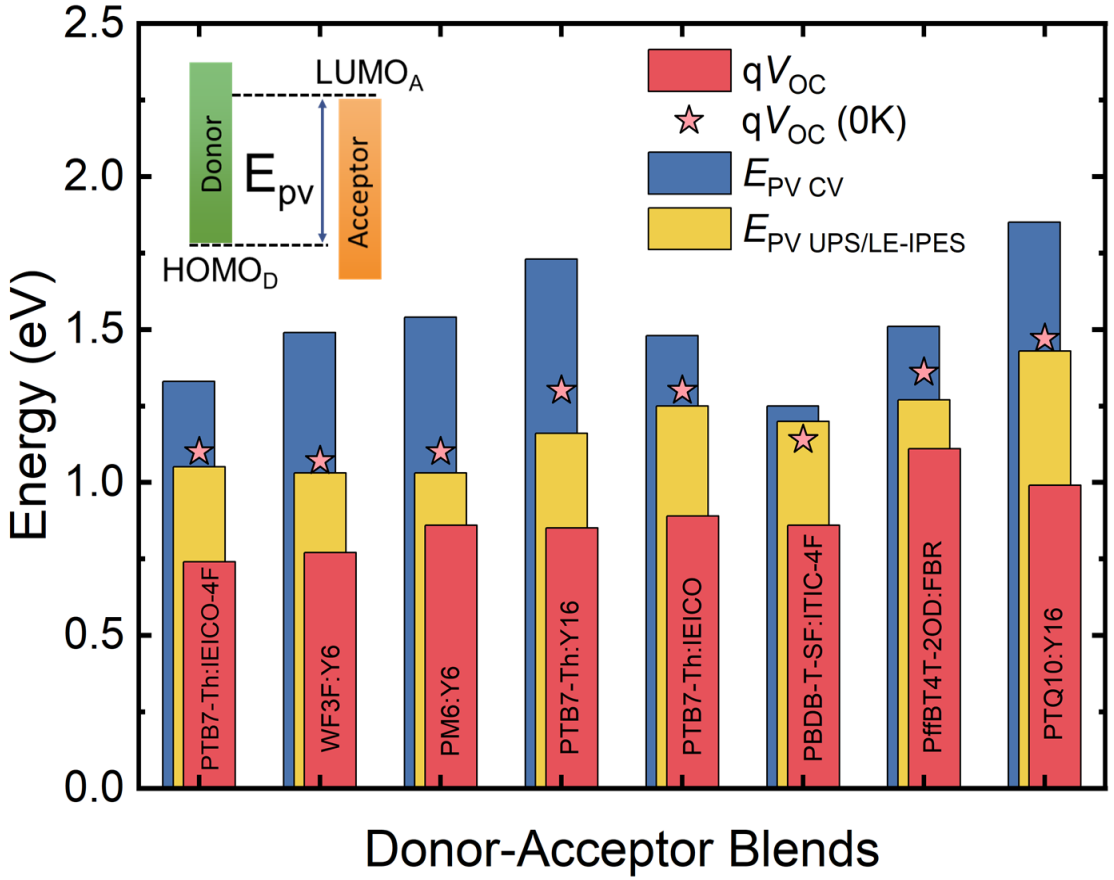
Non-fullerene Acceptors





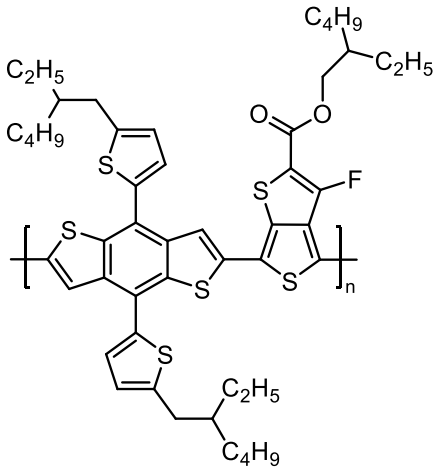
Correlating with IE/EA and Voc



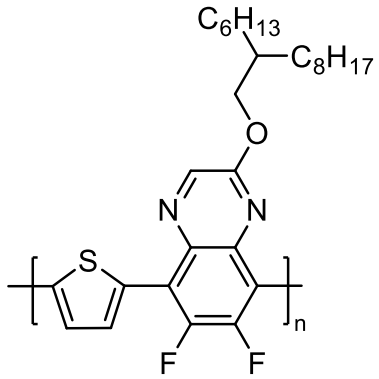


Role of IE-offset in Charge Generation

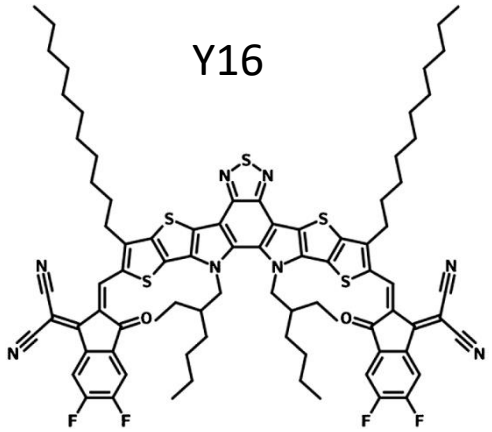
PTB7-Th

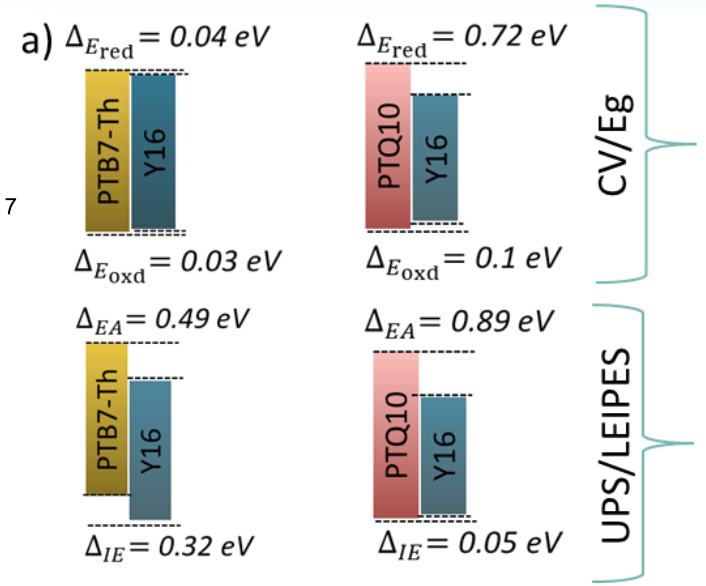


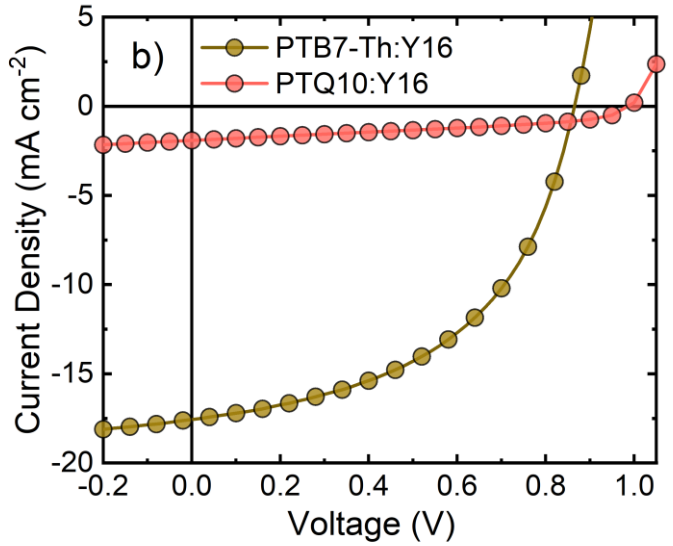
PTQ10

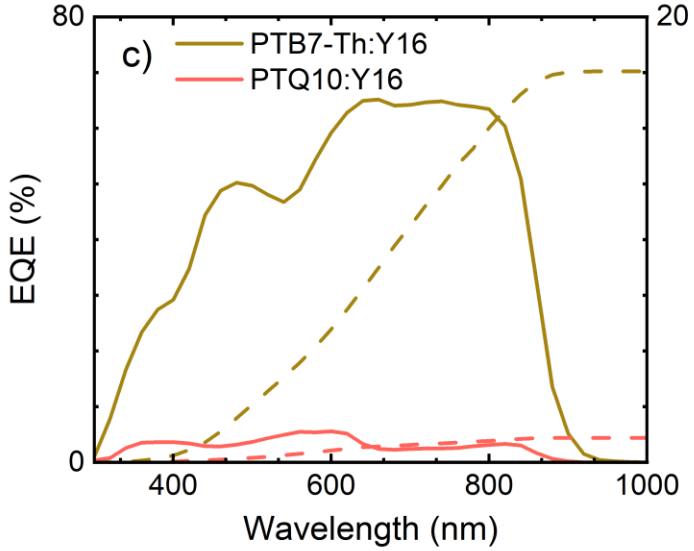


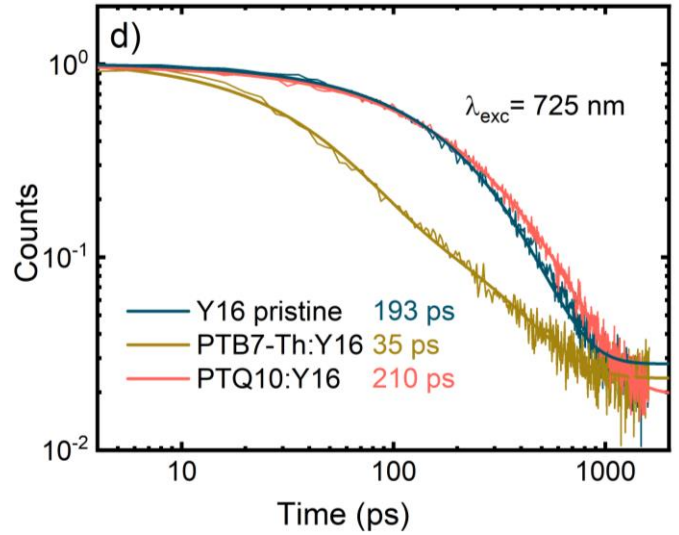
Y16



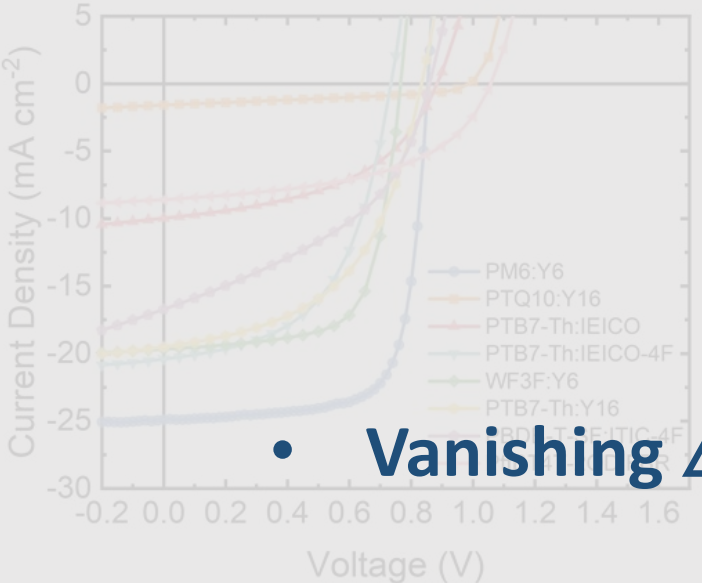








Role of IE-offset in Charge Generation



BHJ Blends	ΔIE_{PES} (eV)	ΔIE_{CV} (eV)	Jsc (mA cm^{-2})	Voc (V)	FF (%)	PCE (%)
PTQ10:Y16	0.05	0.09	1.59	0.99	41	0.64
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	32	0.25
PTQ10:IEICO-4F	0.18	0.06	2.81	0.82	41	0.95
PTQ10:COi8DFIC	0.28	0.13	7.4	0.83	42	2.56
PTB7-Th:Y16	0.31	0.03	19.5	0.87	51	8.3
PTB7-Th:Y1	0.39	0.02	16.6	0.79	40	5.3
PTB7-Th:IEICO-4F	0.45	0.06	20.4	0.74	54	8.1
WF3F:Y6	0.51	0.23	19.7	0.77	68	10.4
PM6:Y6	0.51	0.18	24.9	0.86	70	15

- **Vanishing △IE is <u>DETRIMENTAL</u> For Device Performance**

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King Abdullah University of Science and Technology

KAUST SOLAR CENTER

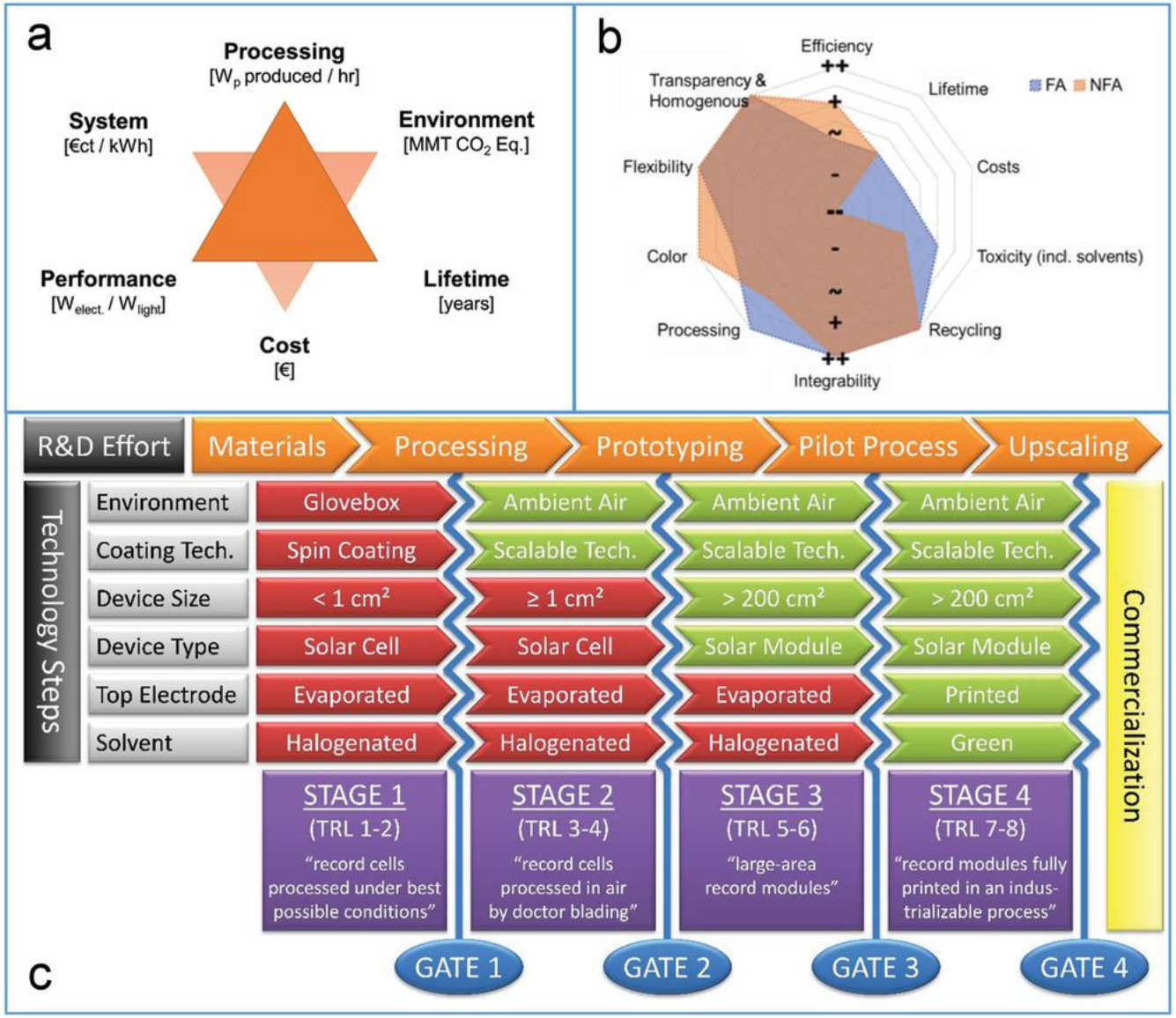
Terpene Based Green Solvents for Stable Organic Photovoltaics

Daniel Corzo

Diego Rosas Villalva

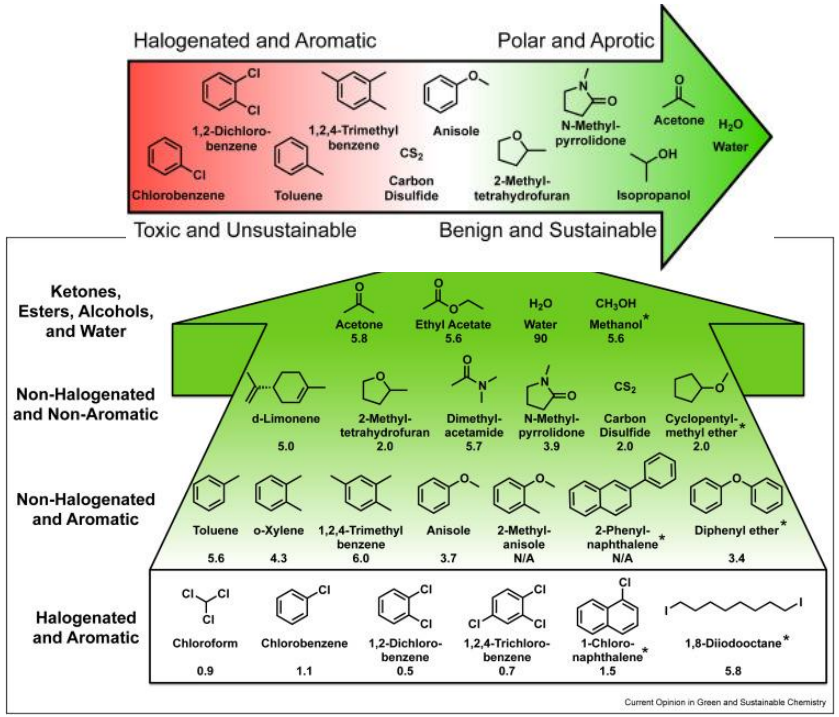
Nature Energy, 2023, 8, 62–73

Opportunities for printed OPV

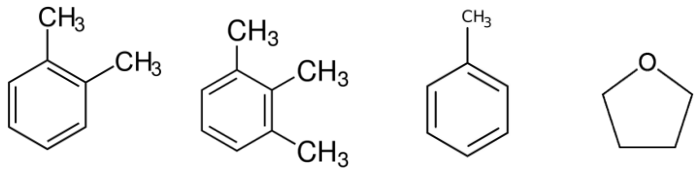


Adv. Energy Mater. 2020, **10**, 2001864

Strategies for green solvent transition

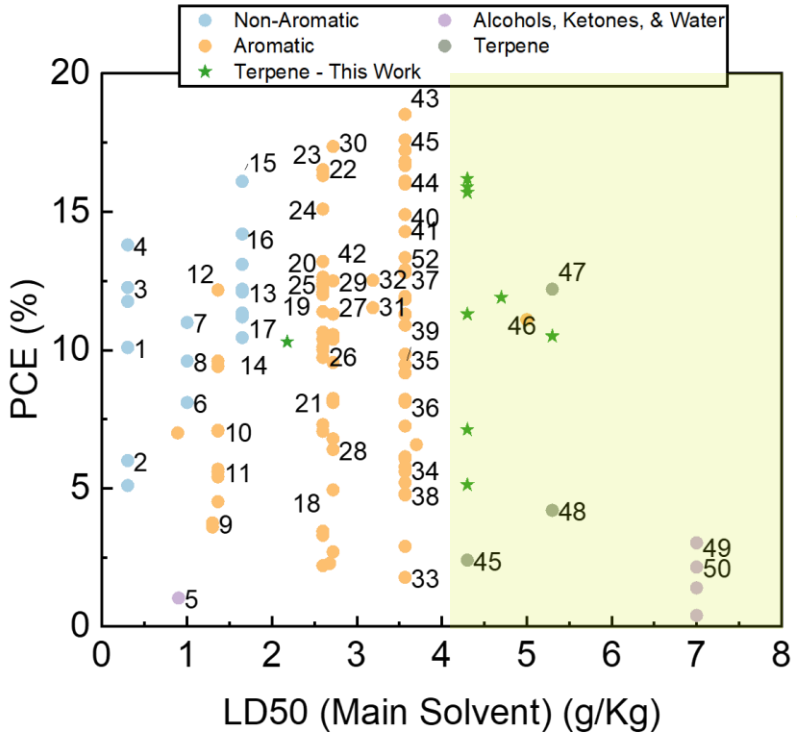


Current Opinion in Green and Sustainable Chemistry 2017, 49-54.
Mater. Today 2016, 553-543

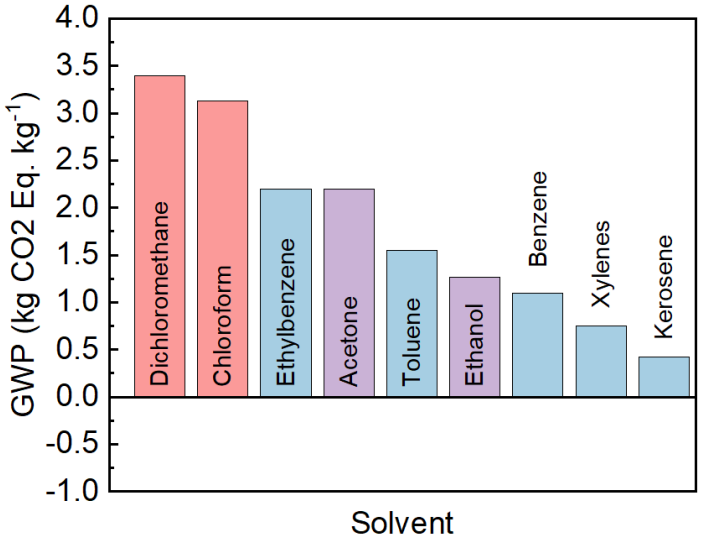


O-xylene TMB Toluene THF

Survey 2013 – 2022



Lethal Dose: is one way to measure the short-term poisoning potential (acute toxicity) of a material.



Ecoinvent LCA Database
Energy Environ. Sci., 2018, 11, 2225-2234

Hansen solubility parameters

Hildebrandt Parameter

$$\delta_T = \sqrt{(E/V)}$$

$$\delta_T^2 = \delta_D^2 + \delta_P^2 + \delta_H^2$$

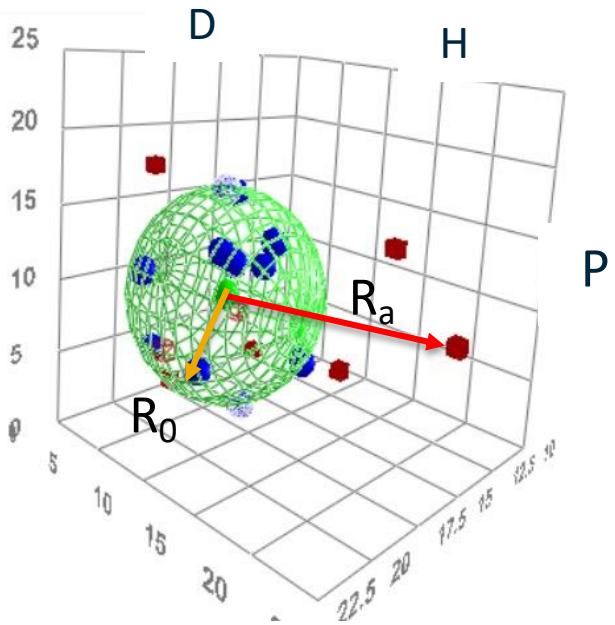
Dispersive **Polar** **Hydrogen bonding**

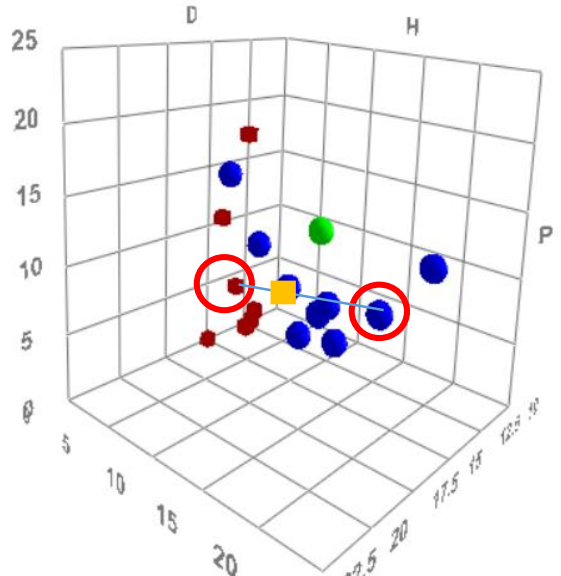
HSP distance - “alikeness”

$$(R_a)^2 = 4(\delta_{D1}-\delta_{D2})^2 + (\delta_{P1}-\delta_{P2})^2 (\delta_{H1}-\delta_{H2})^2$$

HSP linear relationship (mixtures)

$$\delta_{blend} \equiv \left[\varphi_{comp1} \times \sigma_{com1}\right] + \left[\varphi_{comp2} \times \sigma_{com2}\right]$$





Relative Energy Distance = (R_a / R_0)

RED < 1 - Soluble

RED = 1 - P. Soluble

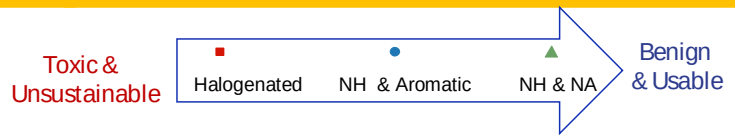
RED > 1 - N. Soluble

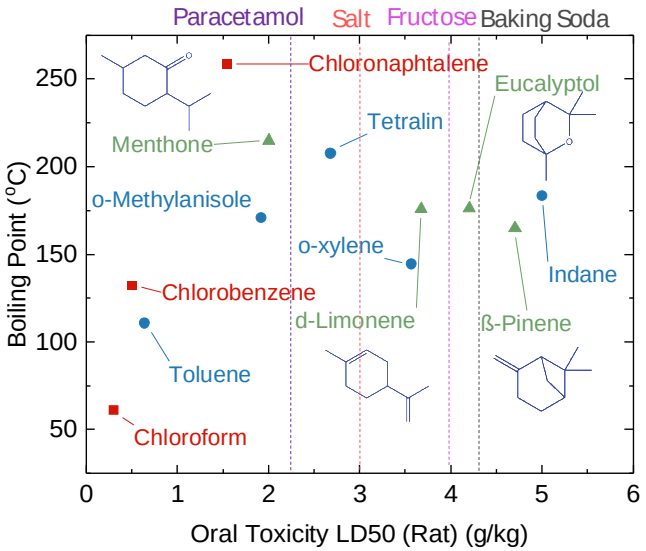
HSPiP

Finding Alternative Solvents

Formulation Guideline

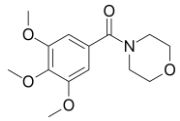
Terpenes as renewable solvents for OPV





Jet Fuel

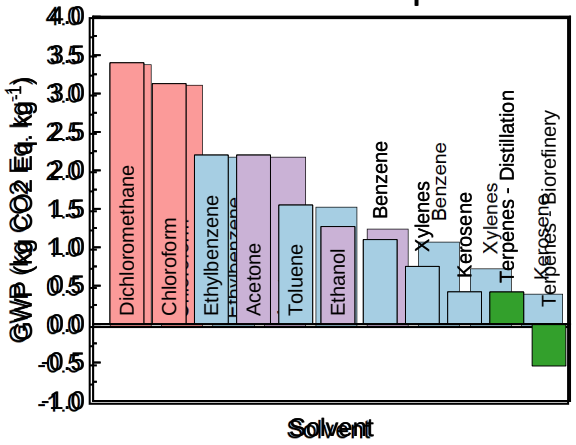
Biopolymers

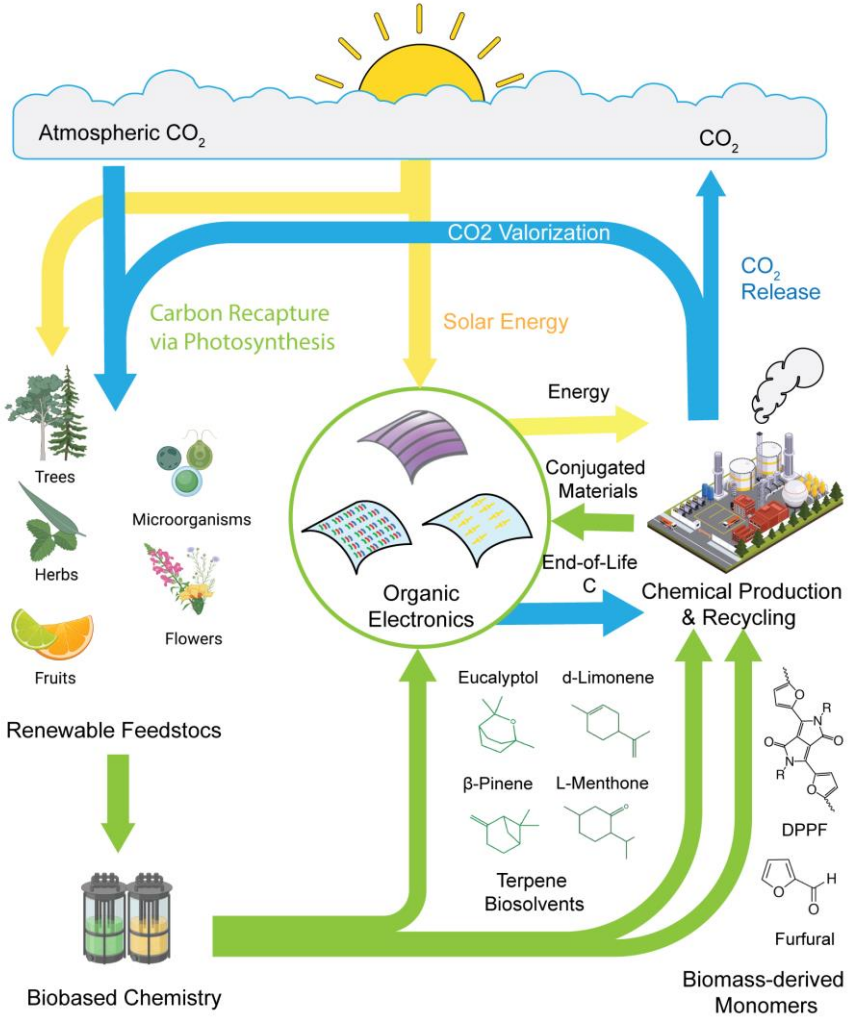


Drug Synthesis

Trends in Biotechnology 35, 227-240
Org. Process Res. Dev. 2020, 24, 11, 2665–2675
Nature Reviews Materials 7, 117-137, (2022)

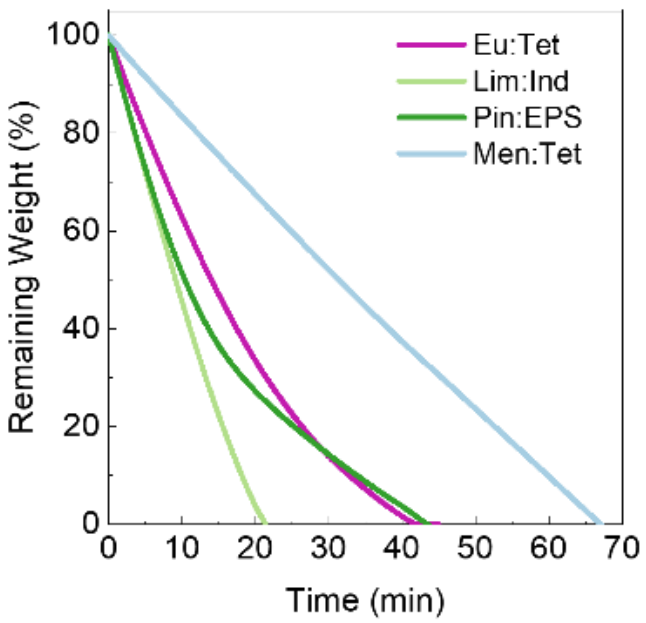
Carbon footprint

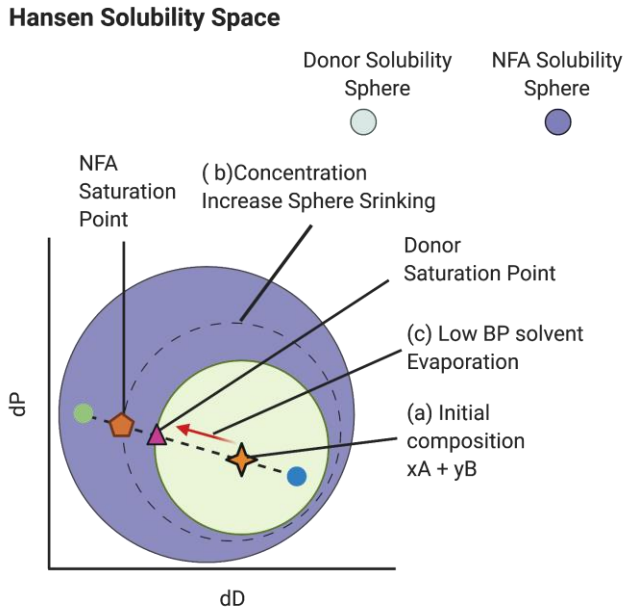


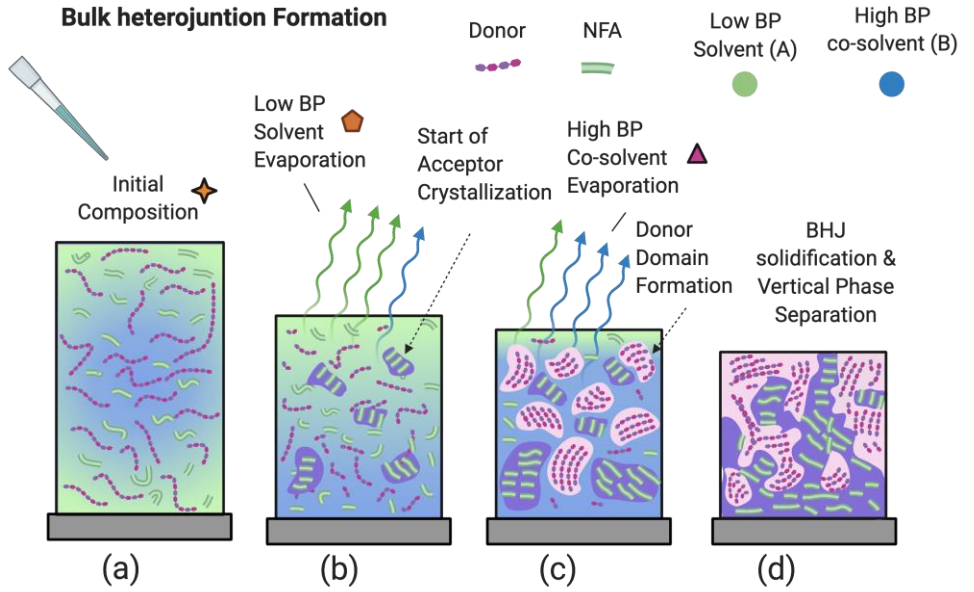


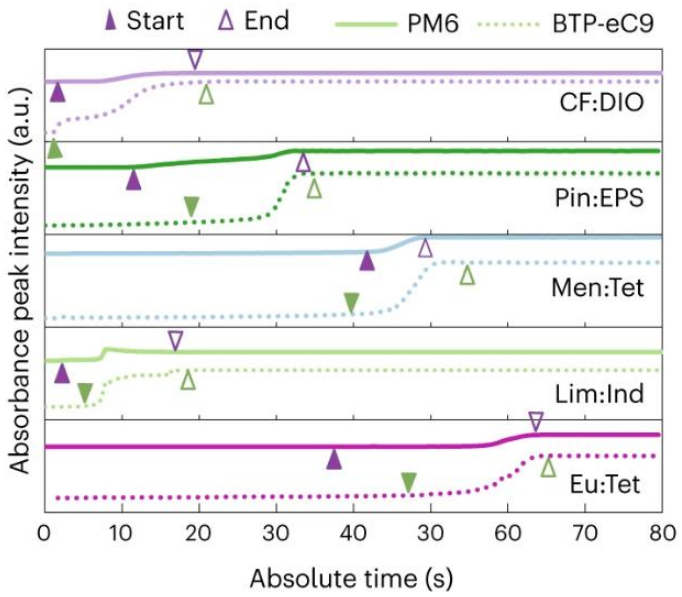
Ecoinvent database
Planta volume 249, pages155–180 (2019)
Industrial & Engineering Chemistry Research 50, 11280-11287
Algal Research 23:1-11 (2017)
Chem. Commun., 2014,50, 15288-15296

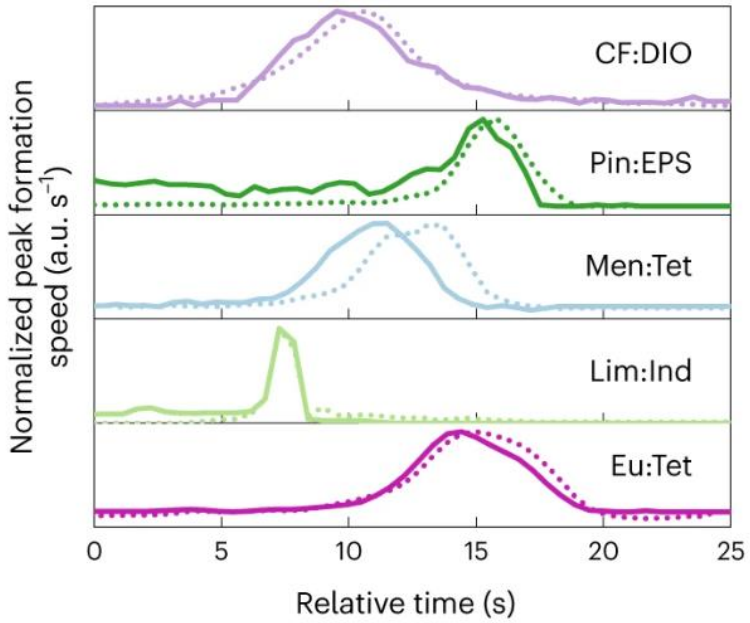
Ink formulation with terpenes



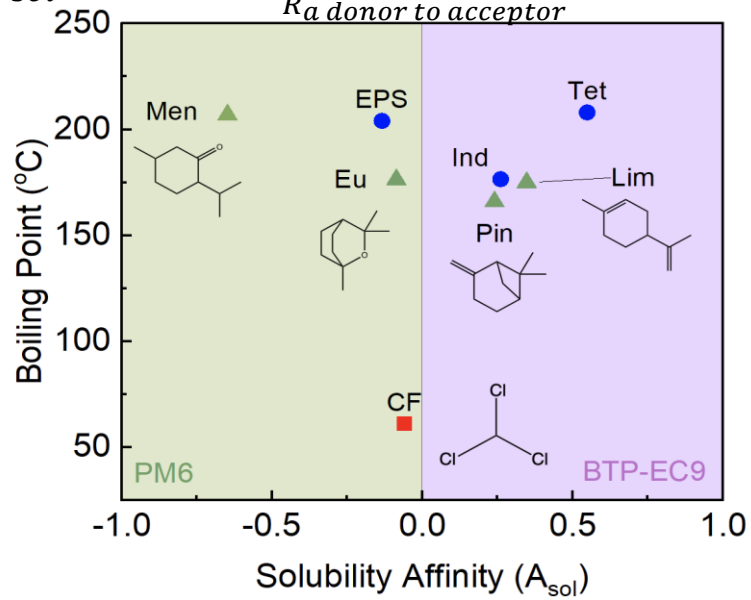




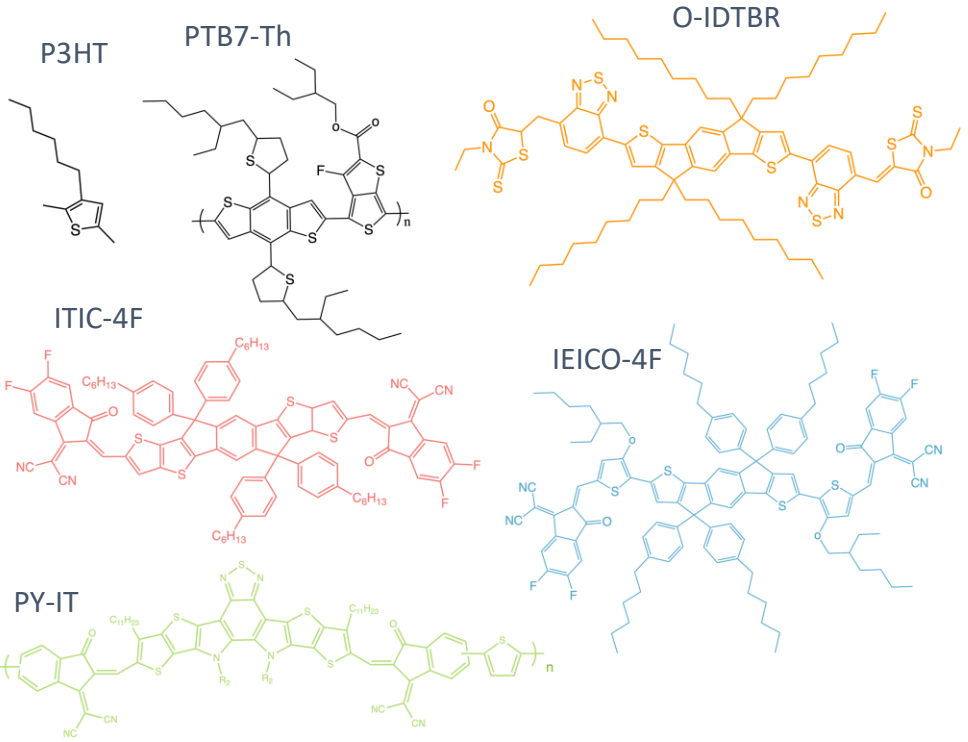




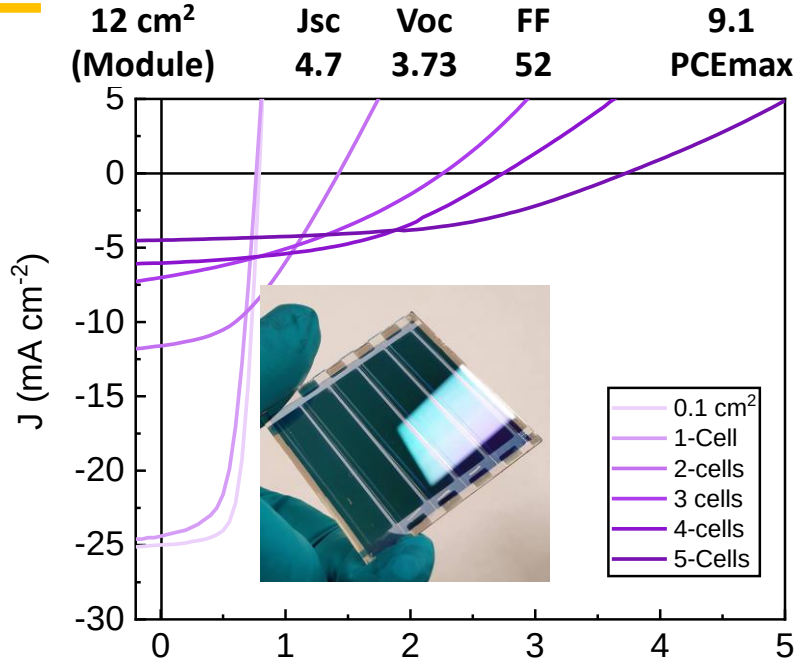
$$A_{sol} = \frac{R_{a\ solvent\ to\ donor} - R_{a\ solvent\ to\ acceptor}}{R_{a\ donor\ to\ acceptor}}$$

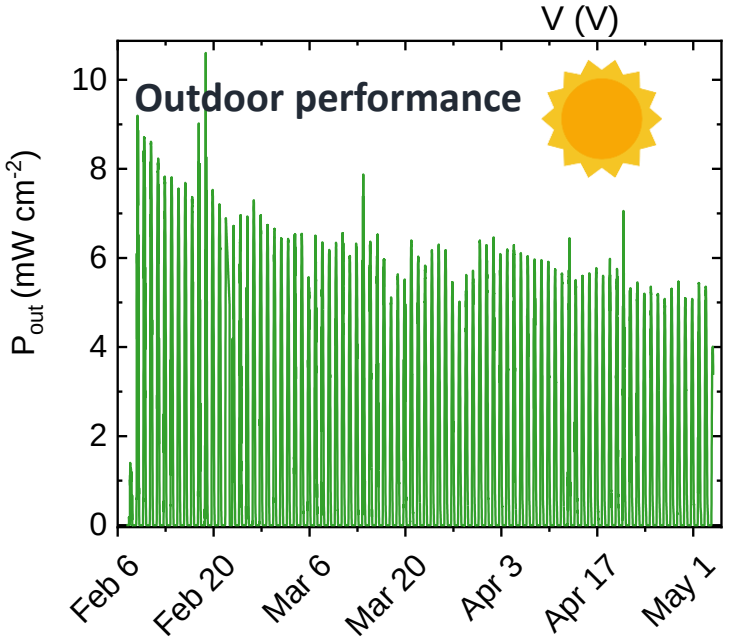


Terpene utilization in NFAs



Blend	J_{sc} (mAcm^{-2})	V_{oc} (V)	FF (%)	PCE_{ave} (%)	PCE_{max} (%)
P3HT:O-IDTBR (1:1)	11.5	0.72	60	5.1%	5.3%
PTB7-Th:IEICO-4F (1:1.5)	24.7	0.69	59	9.8%	10.6%
PM6:IT-4F (1:1.2)	15.2	0.81	55	6.8%	7.3%
PM6:PY-IT (1:1.2)	23.8	0.92	72	15.7%	15.9%
PM6:(PY-IT:BTP-eC9) (1:0.9:0.1)	25.5	0.89	71	16.1%	16.3%

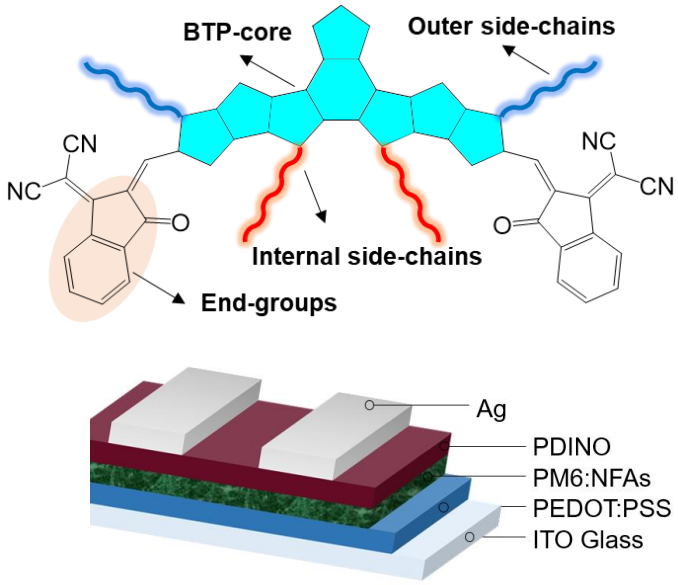




Environment	Ambient Air
Coating Tech.	Scalable
Device Size	12cm²
Device Type	Module
Top Electrode	Evaporated
Solvent	Green Solvents

Stability of Y-NFAs

Optimized using No solvent additives



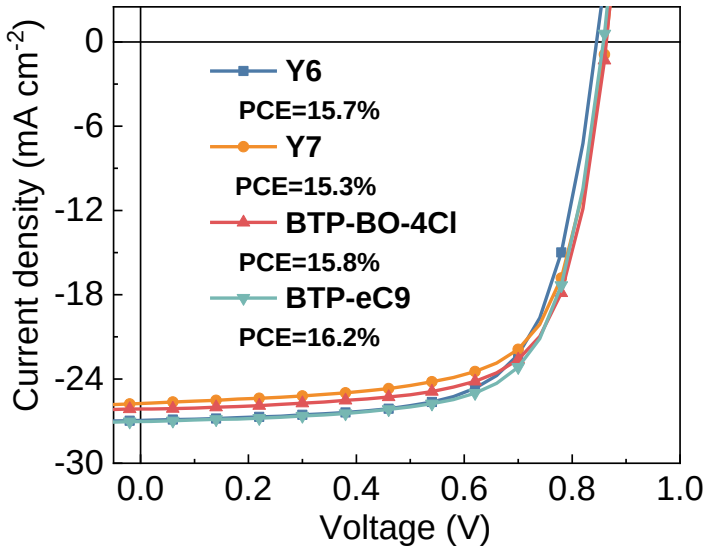
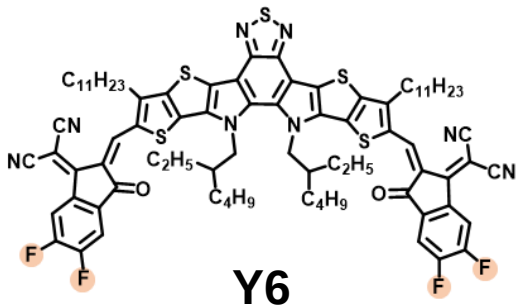
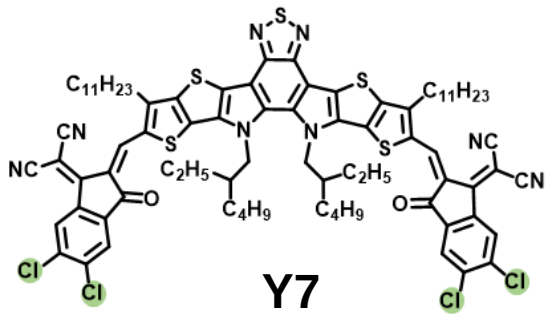


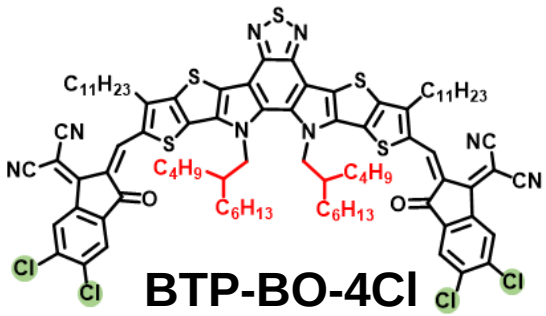
Table. Photovoltaic parameters of the devices

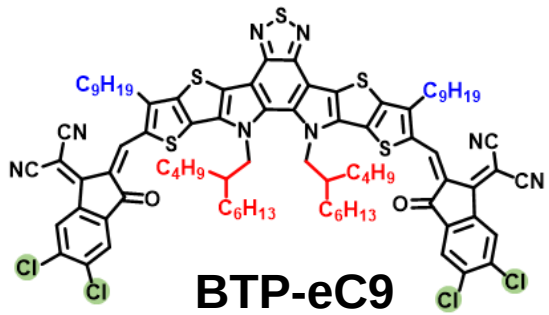
Acceptor[a]	J_{SC} (mA cm^{-2})	V_{OC} (V)	FF (%)	PCE (%)
Y6	26.9	0.85	68.9	15.7
Y7	25.7	0.86	69.0	15.3
BTP-BO-4Cl	26.1	0.86	70.1	15.8
BTP-eC9	27.0	0.86	69.9	16.2

[a] PM6:Y6=1.1.2, 100 °C annealing 10 min, w/o additive









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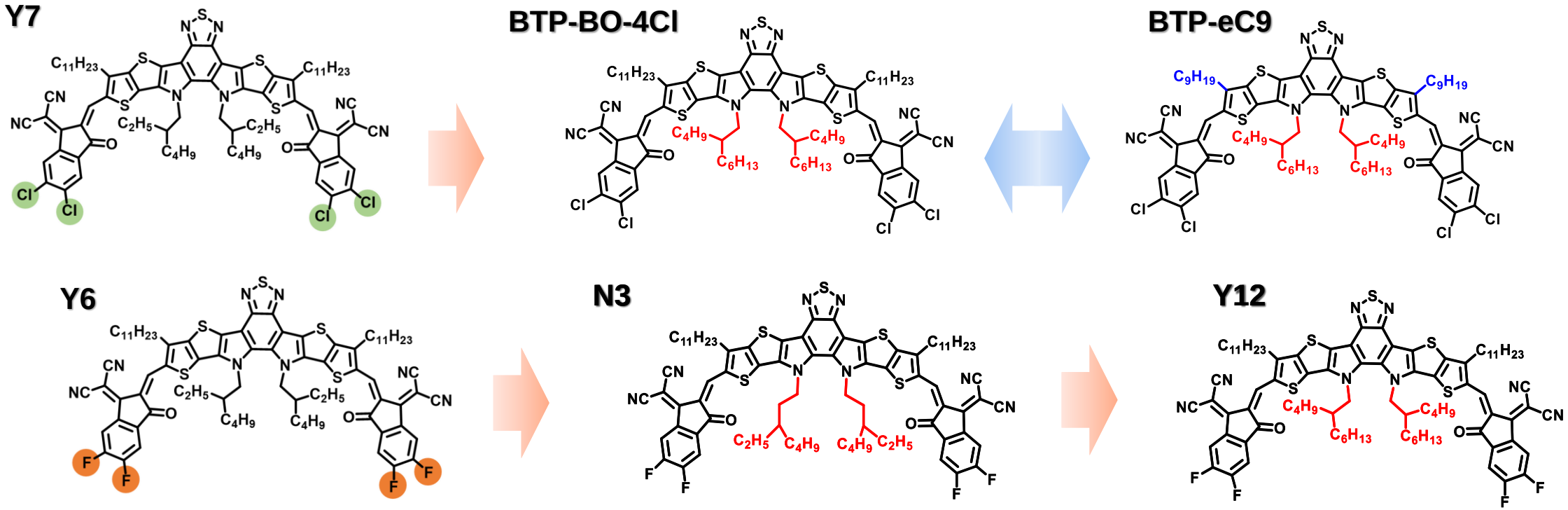
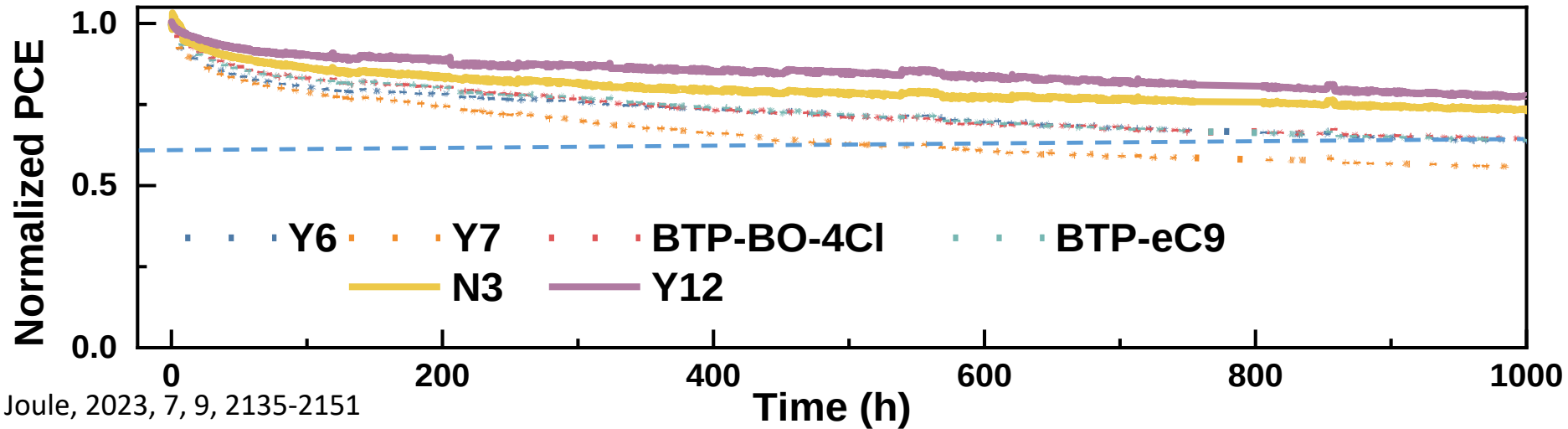
Structure-stability relationship of Y-NFAs





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