Single-Component Organic Solar Cells: Efficiency, stability, and industrial viability

Yakun He

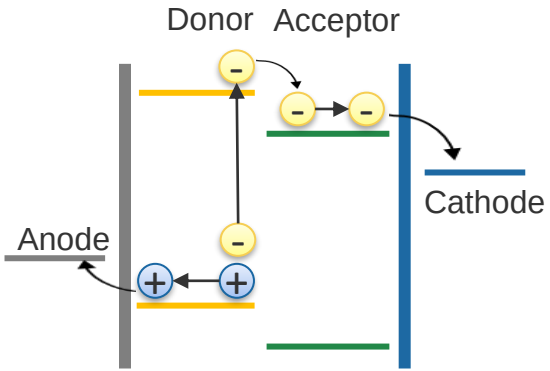
KAUST Global Fellowship Postdoc
King Abdullah University of Science and Technology (KAUST, Saudi Arabia)
Prof. Frédéric Laquai

Date: 22/05/2024

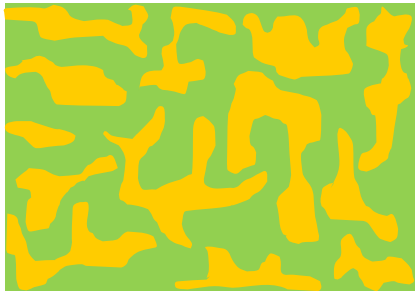
Organic solar cells

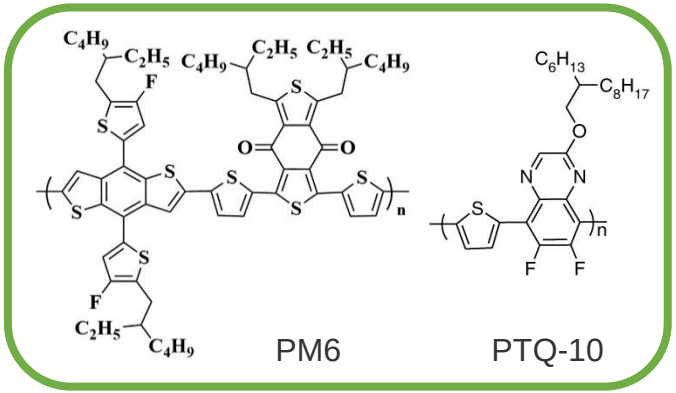
Pictures from Internet, COP26, OPVIUS, Heliatek, ASCA-ARMOR, KAUST.

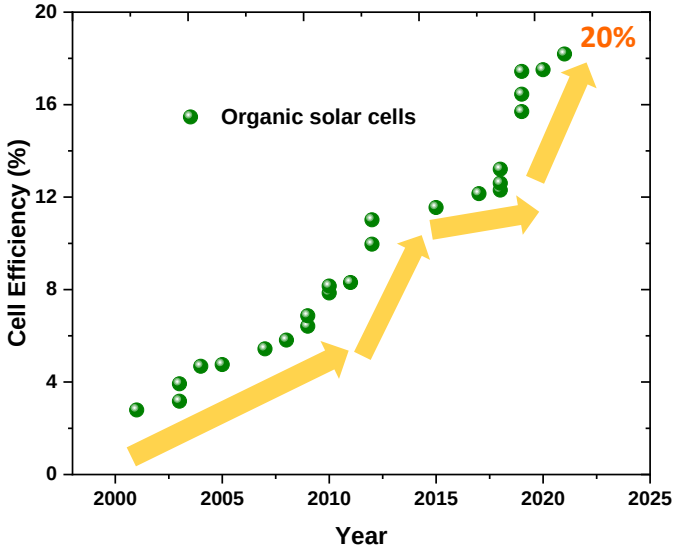
Organic solar cells

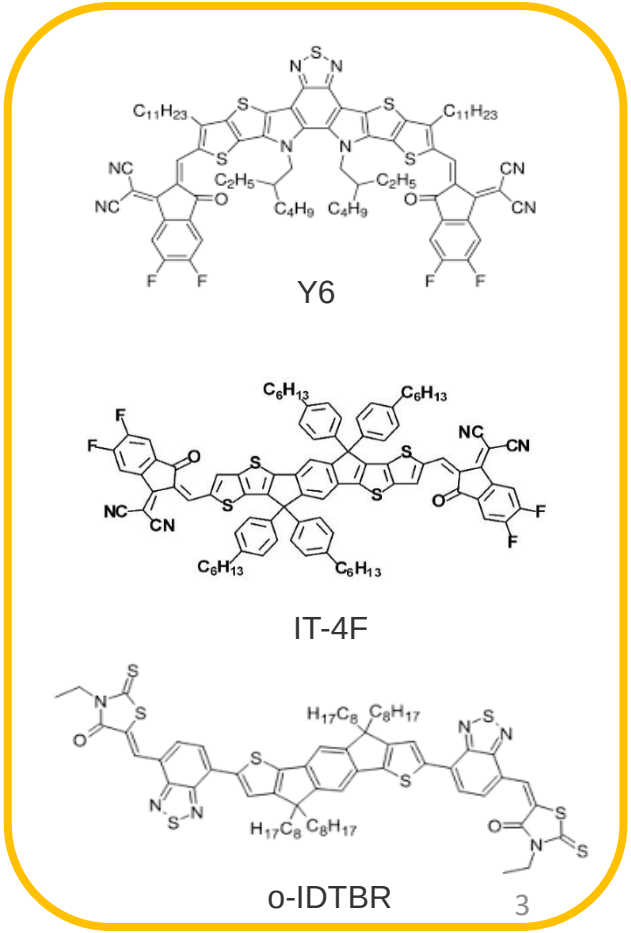


Bulk Hetero-Junction (BHJ)



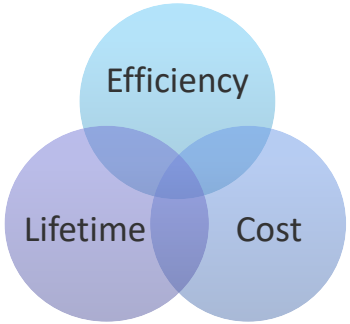


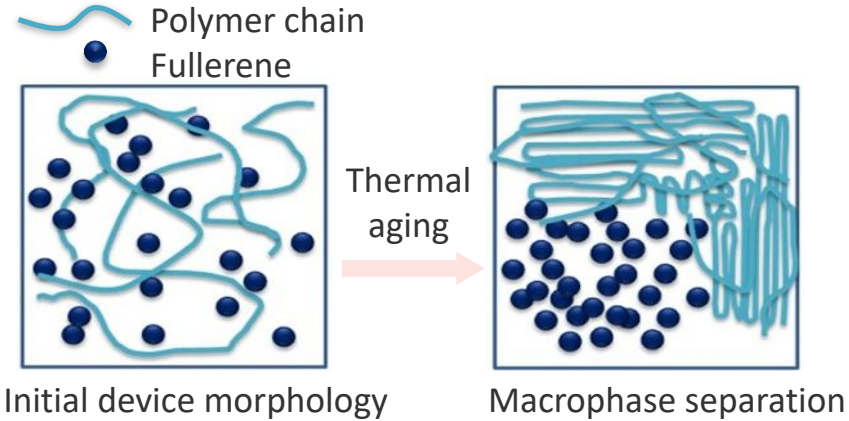


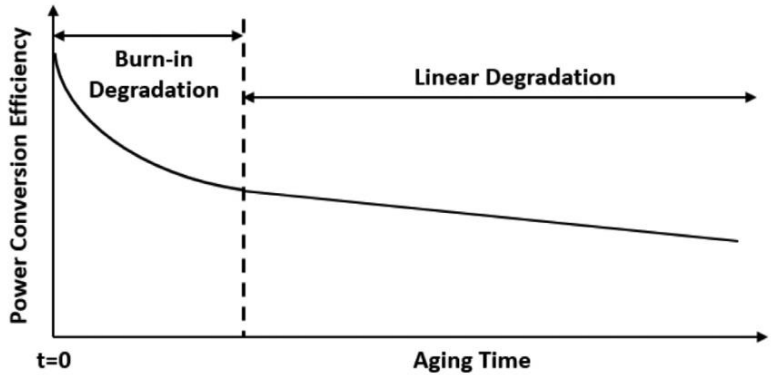


NREL.

Organic solar cells

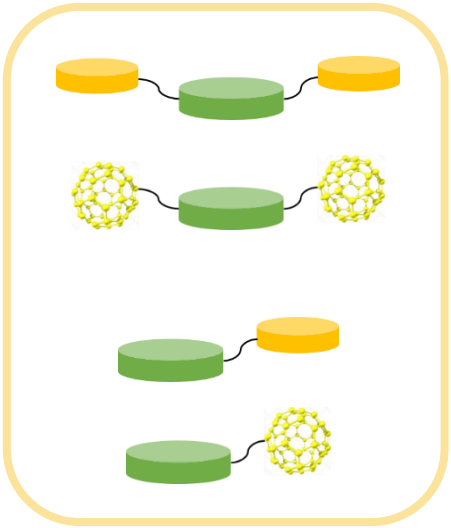




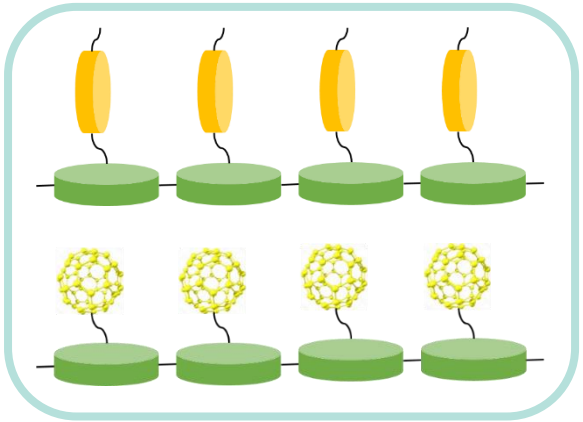


J.W. Rumer, I. McCulloch, Materials Today, 2015, 18, 425-435; L. Duan, et al. Adv. Sci., 201903259.

Single-component materials



Molecular dyads and triads



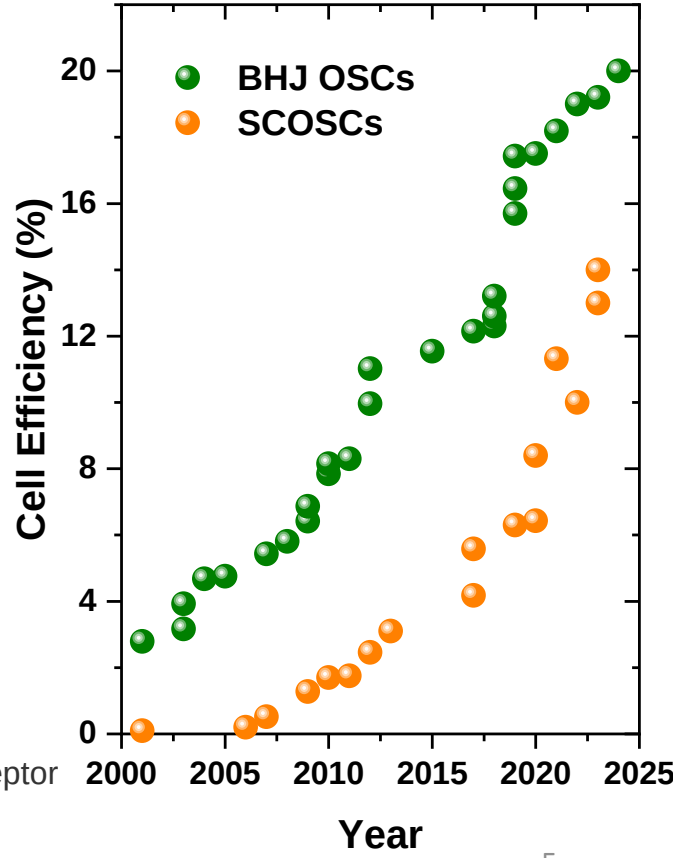
Polymers (side-chain)

Polymers (in-chain)

Donor

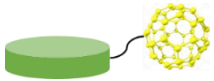
Non-fullerene acceptor

Fullerene acceptor



Y.K. He, N. Li, C.J. Brabec et al. Joule 2022.

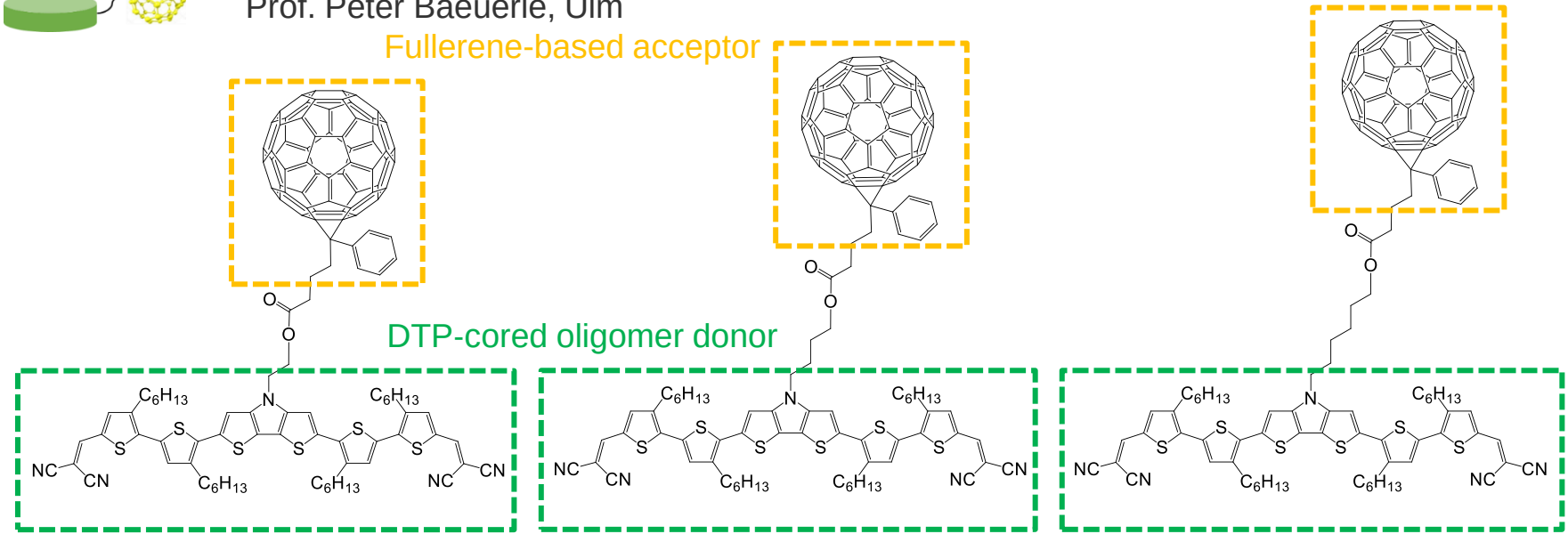
Molecular dyads



Prof. Peter Baeuerle, Ulm

Fullerene-based acceptor

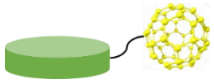
DTP-cored oligomer donor



dyad **1**, **2**, **3** PCE = 4.21%, 2.74%, 3.34%

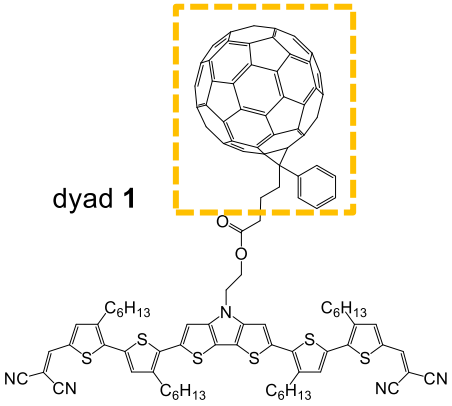
S. Lukas et al. Chem. Commun., 2019, 55, 14202-14205; S. Lukas et al. Solar RRL, 202000653

Molecular dyads



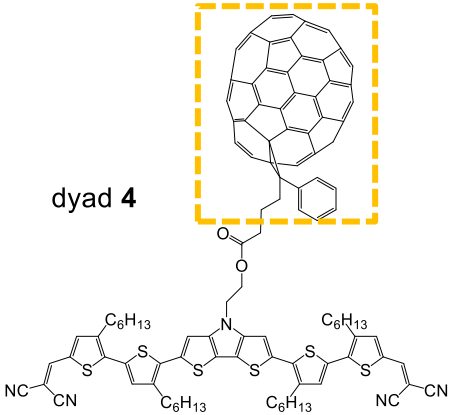
Prof. Peter Baeuerle, Ulm

dyad **1**

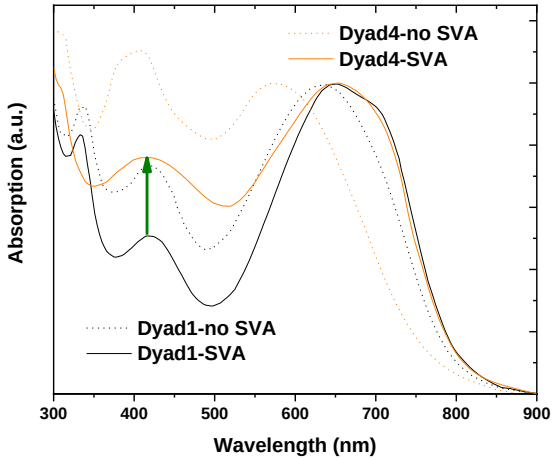


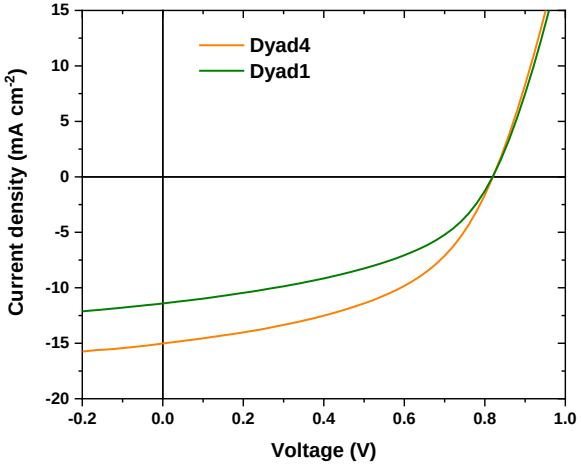
PCE = 4.21%

dyad **4**



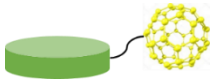
PCE = 5.34%



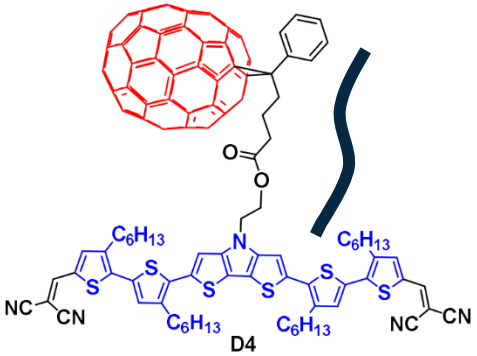


A. Aubele, Y.K. He, et al. Adv. Mater., 2021, 2103573.

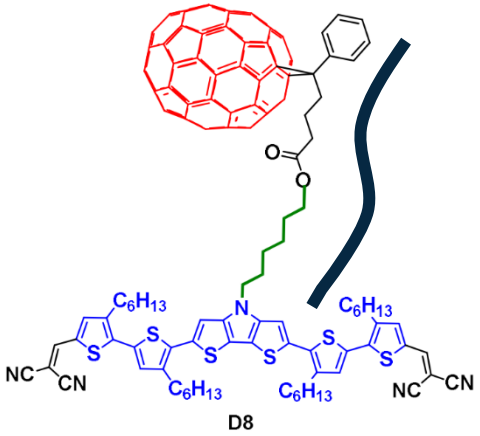
Molecular dyads



PCE = 1.78%
SVA 30 s

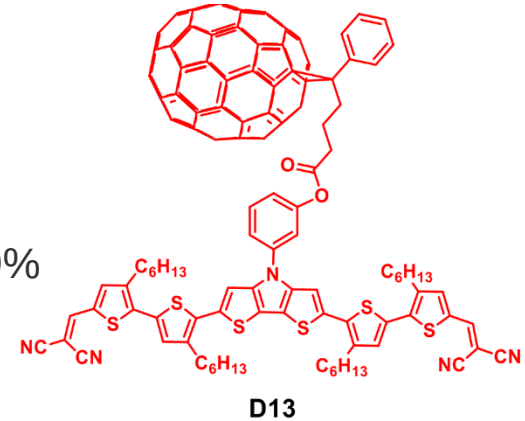


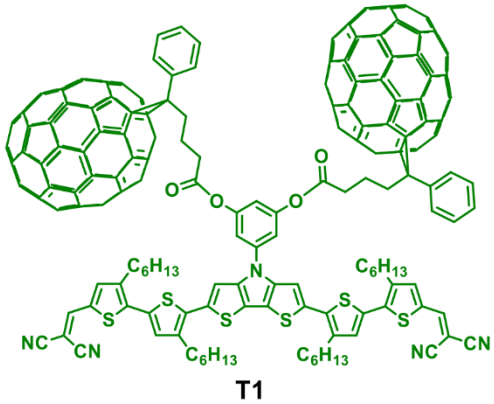
PCE = 5.34%
SVA 25 s



PCE = 4.3%
SVA 20 s

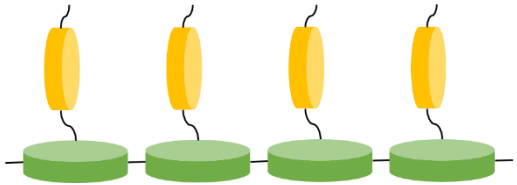
PCE = 2.79%
SVA 20 s





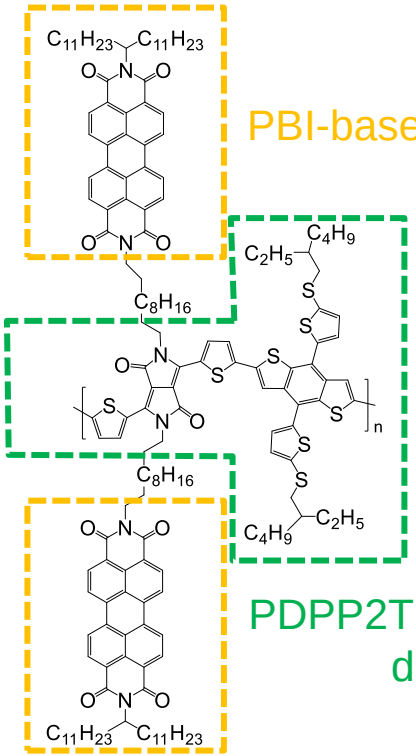
PCE = 4.61%
SVA 40 s

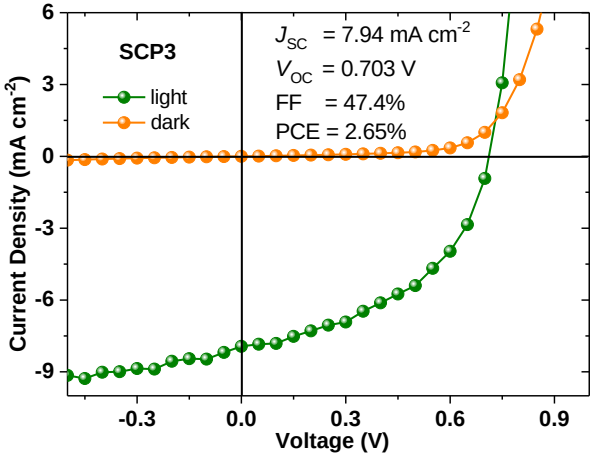
Polymers (side chain)



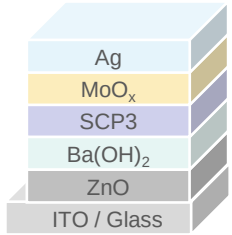
Double-cable polymers

Prof. Weiwei Li
Beijing





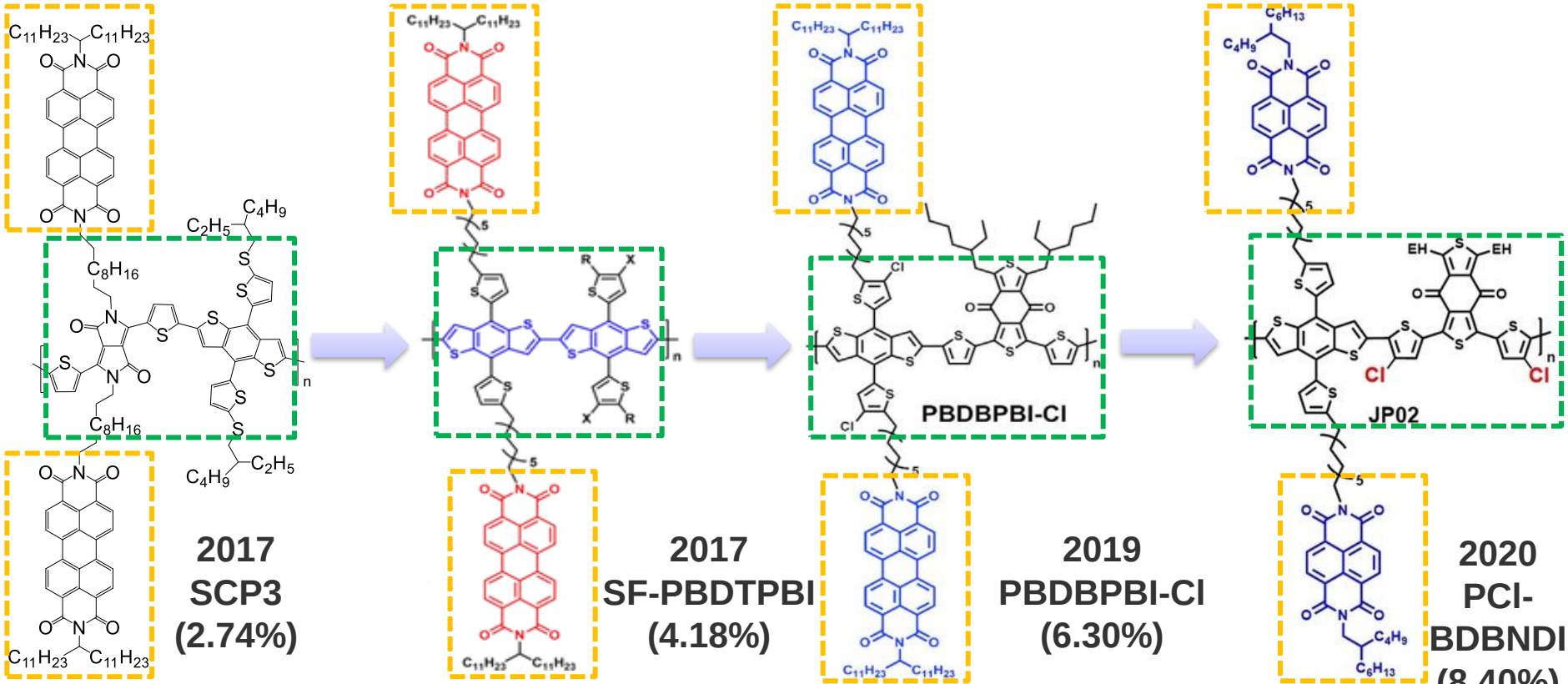
PCE = 2.65%



W.B. Lai, W.W. Li, et al. Chem. Mater. 2017, 29, 17, 7073-7077

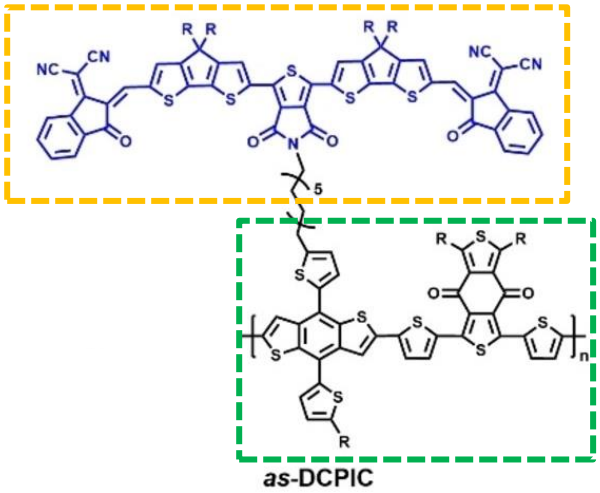
Polymers (side chain)

Double-cable polymers

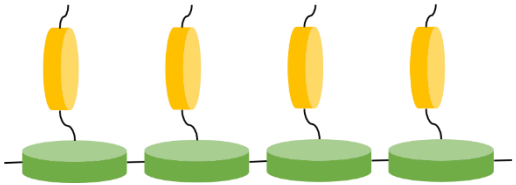


W. Lai, et al. Chem. Mater. 2017, 29, 7073–7077; G. Feng, et al., J. Am. Chem. Soc. 2017, 139, 18647–18656; G. Feng, et al., Joule 2019, 3, 1765–1781; X. Jiang, et al., Angew. Chemie 2020, 132, 21867–21876.

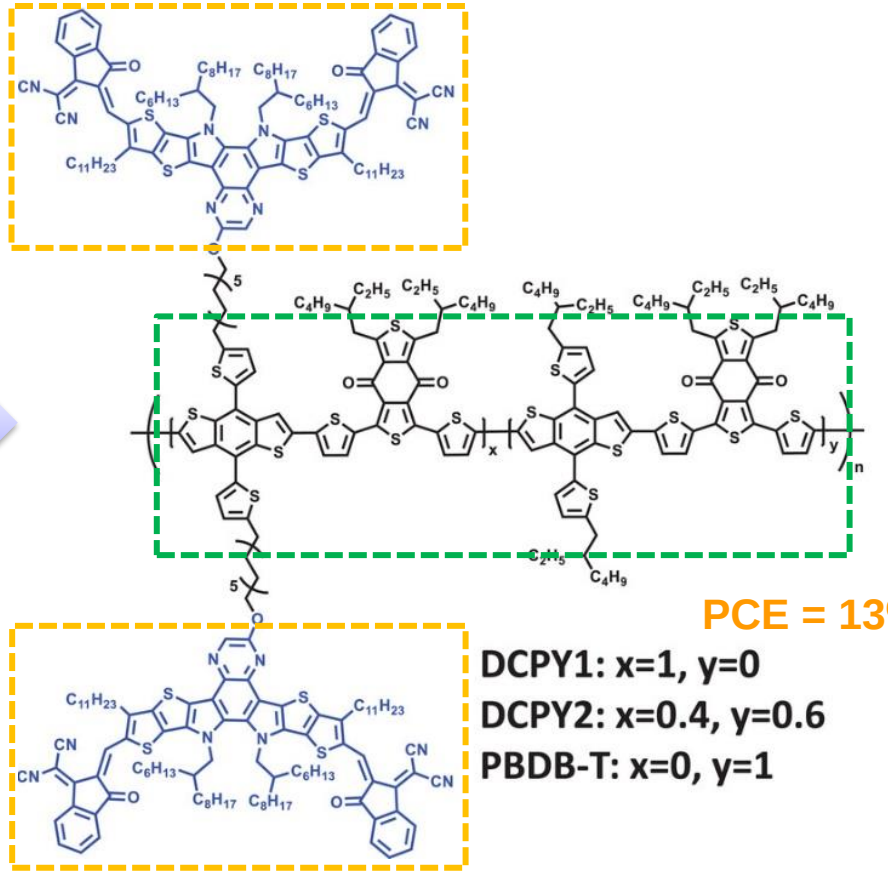
Polymers (side chain)



PCE = 10%



Double-cable polymers



PCE = 13%

DCPY1: x=1, y=0

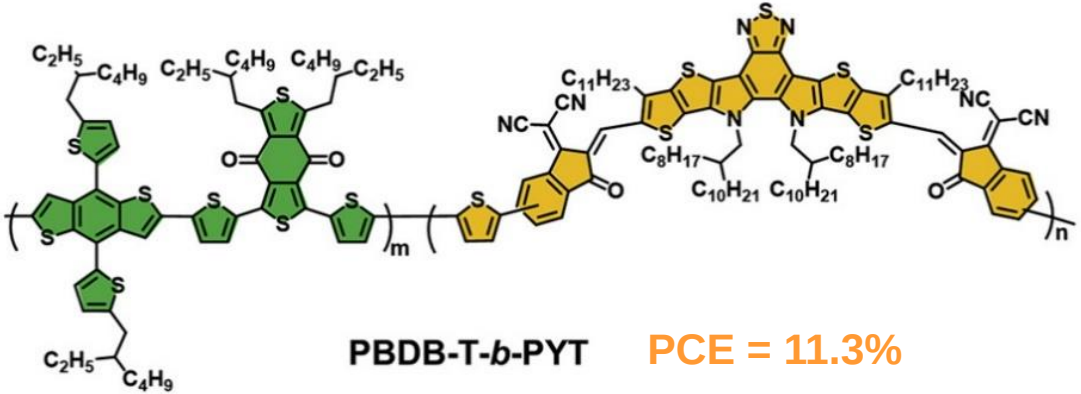
DCPY2: x=0.4, y=0.6

PBDB-T: x=0, y=1

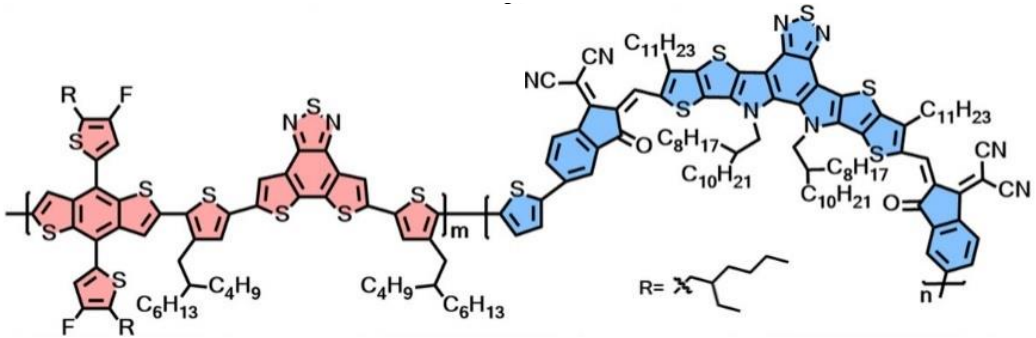
Angewandte Chemie, 202209316; Adv. Mater, 202300629

Polymers (in chain)

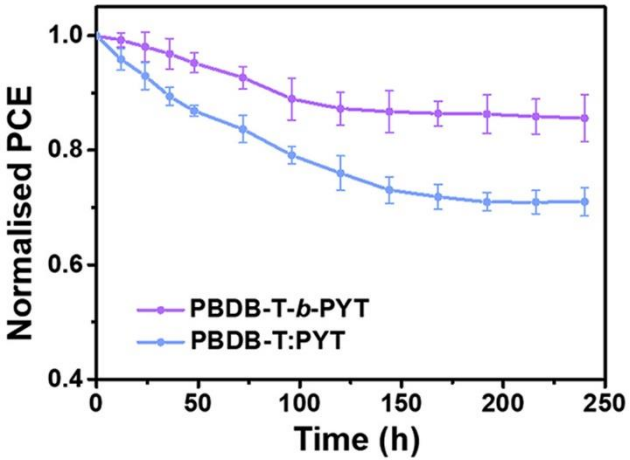
Diblock copolymers

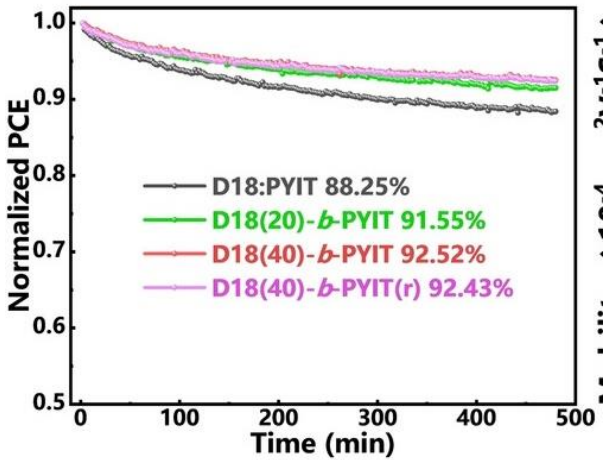


PBDB-T-*b*-PYT PCE = 11.3%



D18-*b*-PYIT PCE = 13.4%





Joule, 5, 2021, 1800-1815; Angewandte Chemie, 202308267

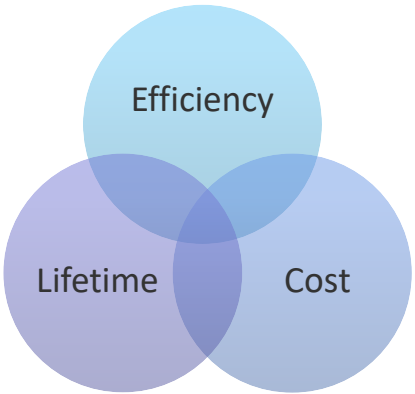
Industrial figure of merit (i-FoM)

$$\mathrm{i-FoM} = \frac{PCE \times photostability}{Synthetic\ complexity}$$

PCE: initial PCE value at time 0

Photostability: percentage left after aging for 200 h

$$SC = 35\frac{NSS}{NSS_{max}} + 25\frac{\log(RY)}{\log(RY_{max})} + 15\frac{NUO}{NUO_{max}} + 15\frac{NCC}{NCC_{max}} + 10\frac{NHC}{NHC_{max}}$$



NSS: number of synthetic steps

RY: (reciprocal) yields of the monomers

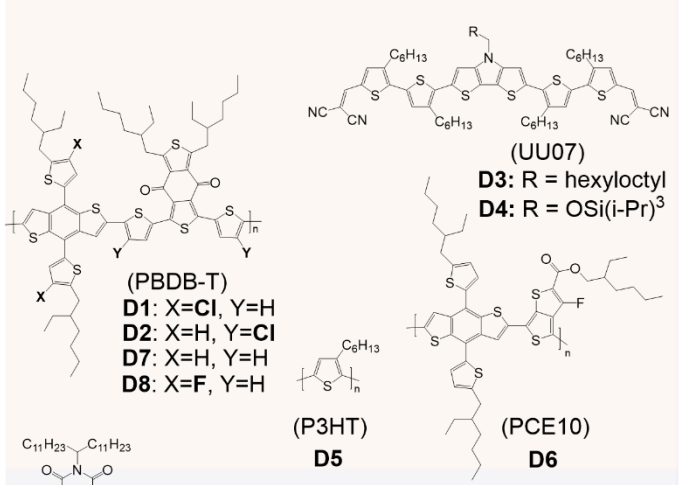
NUO: number of unit operations

NCC: number of column chromatography required for the purification of the monomers

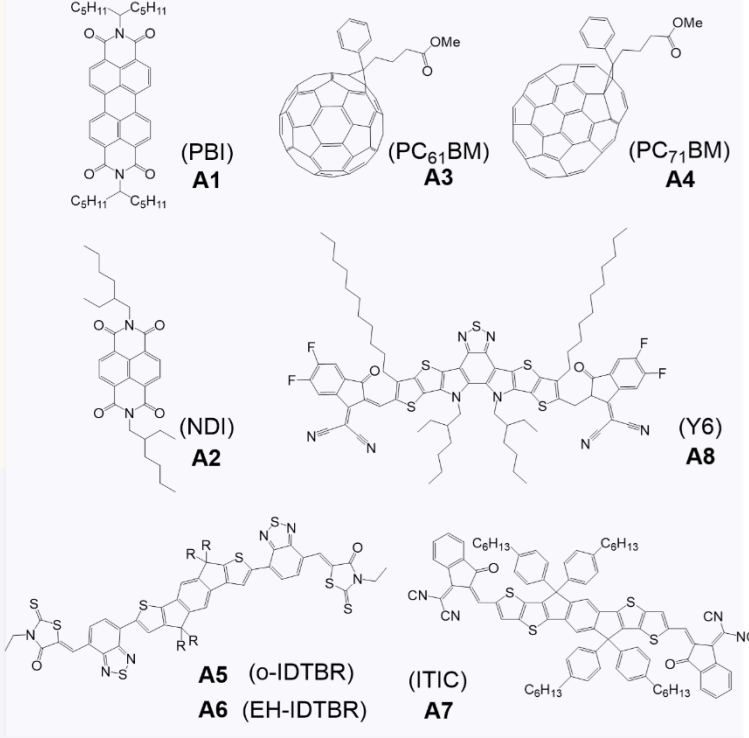
NHC: number of hazardous chemicals used

Y.K. He, N. Li, C.J. Brabec et al. Joule 2022 ; Po et al. Macromolecules 2015, 48, 453–461.

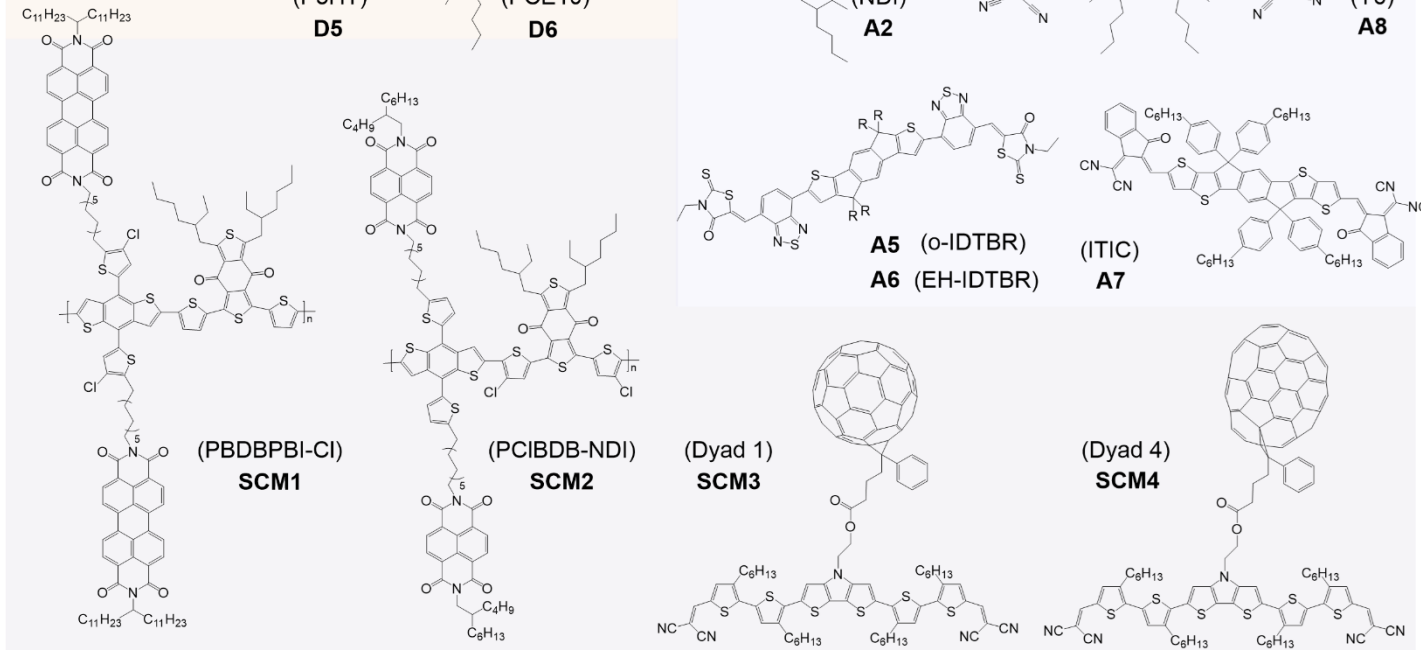
Donors



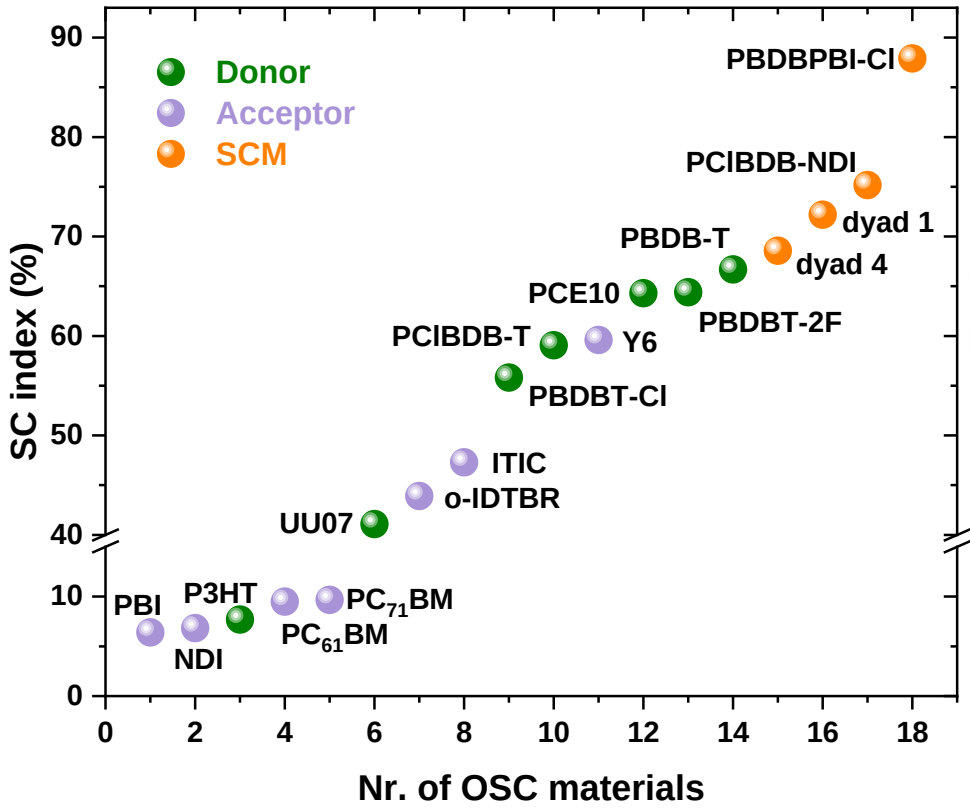
Acceptors

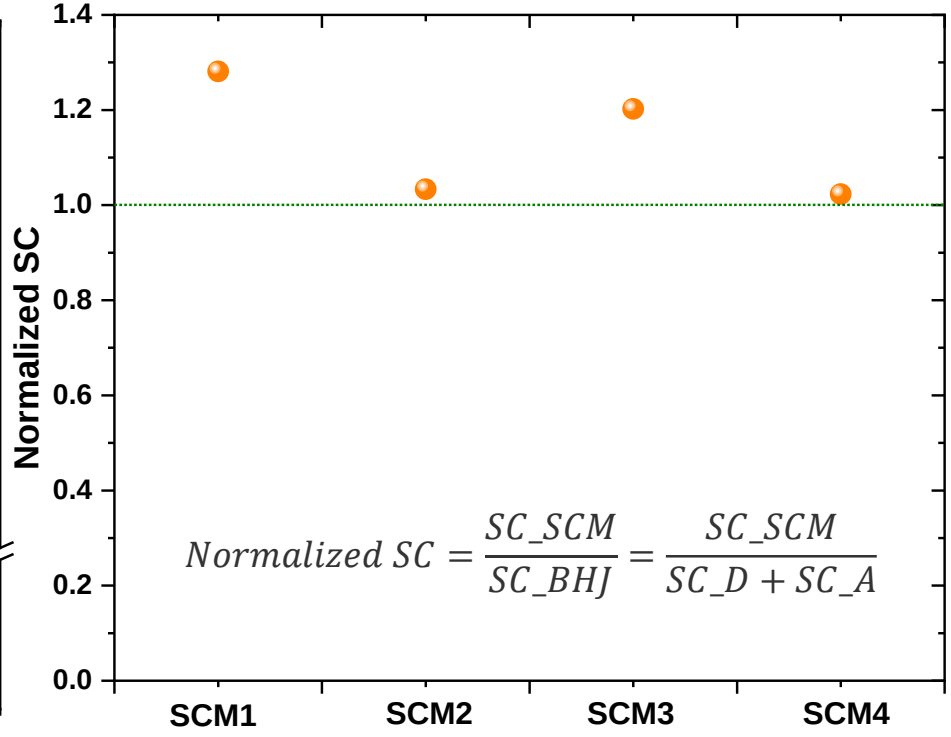


Single Component Materials



Synthetic complexity (SC)

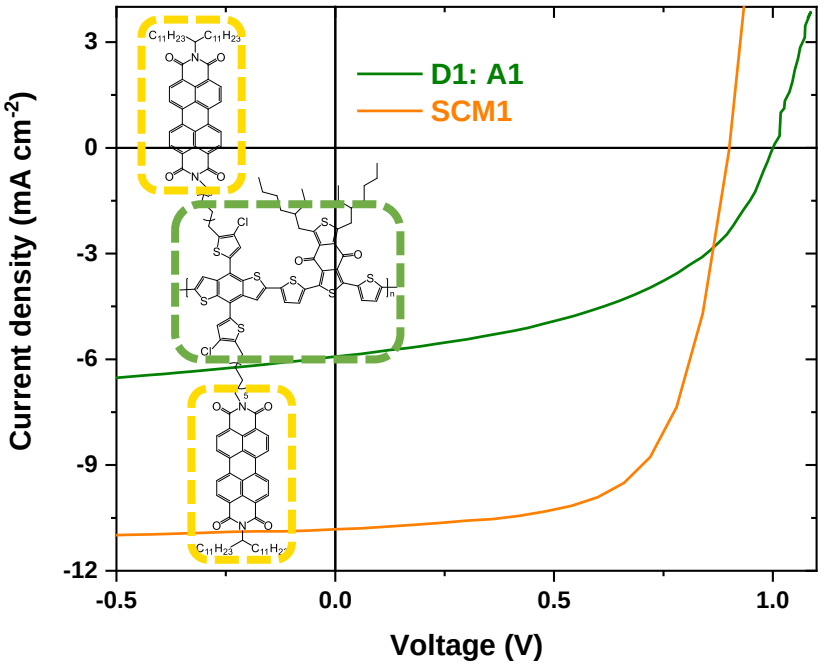




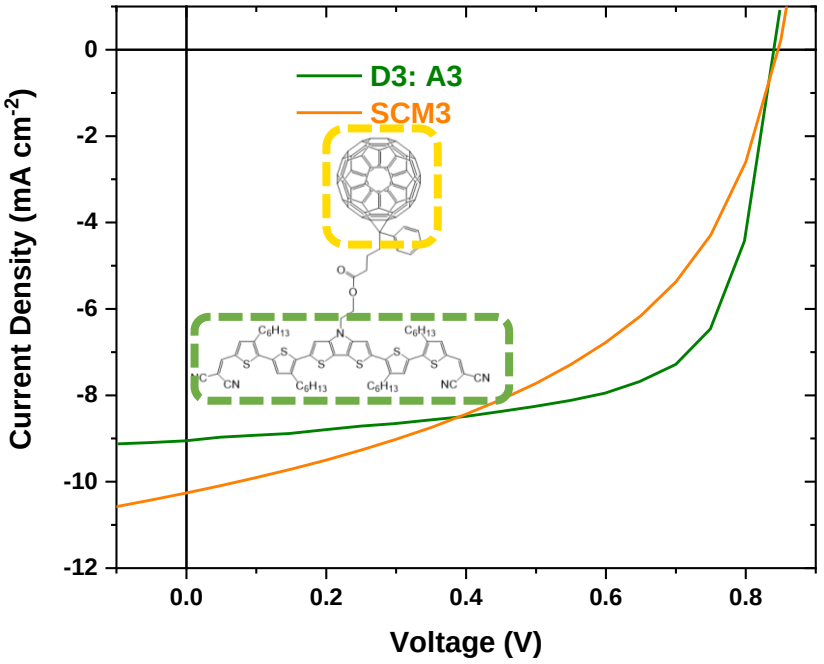
- How much more complex of SCMs than BHJ?
- around 20%.

Y.K. He, N. Li, C.J. Brabec et al. Joule 2022

PCE

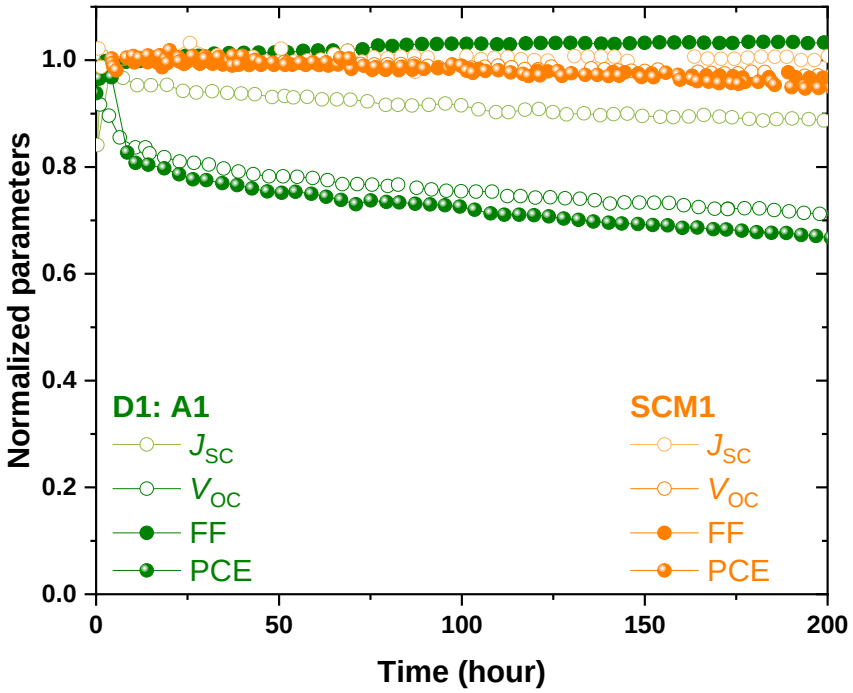


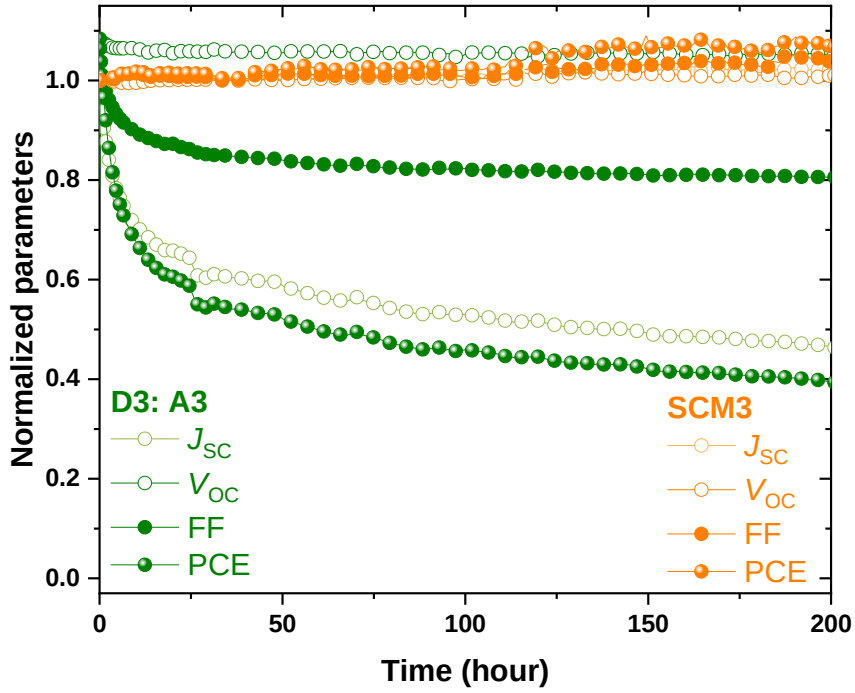
- SCM1 higher PCE
- Overcome incompatibility of D1:A1
- Without excessive phase separation



- SCM3 slightly lower (**comparable**) PCE
- Different morphology
- Generation and recombination: fill factor

Photostability

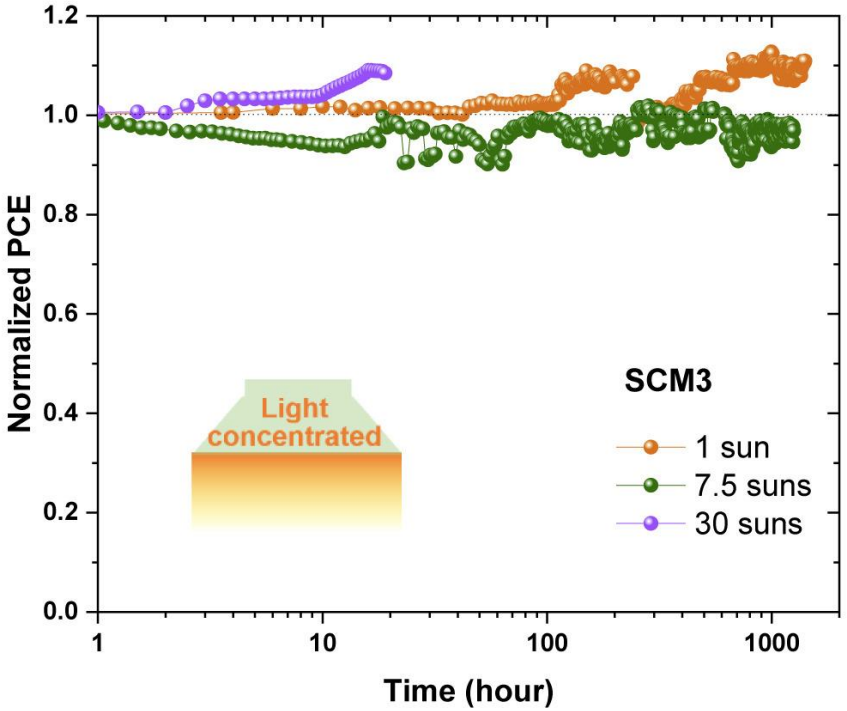


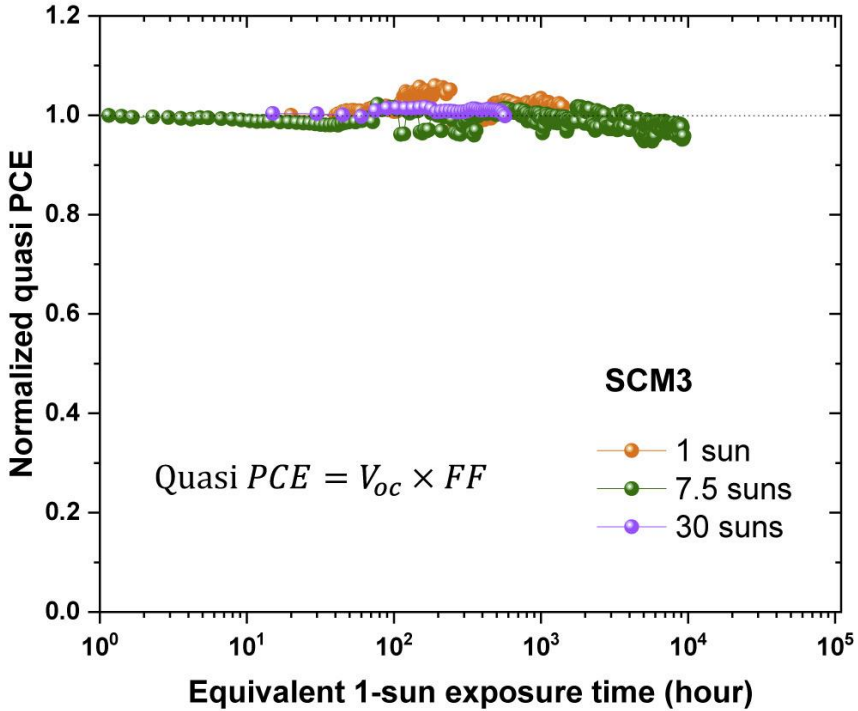


SCMs show enhanced stability than the corresponding BHJs

Y.K. He, N. Li, C.J. Brabec et al. Joule 2022

Photostability

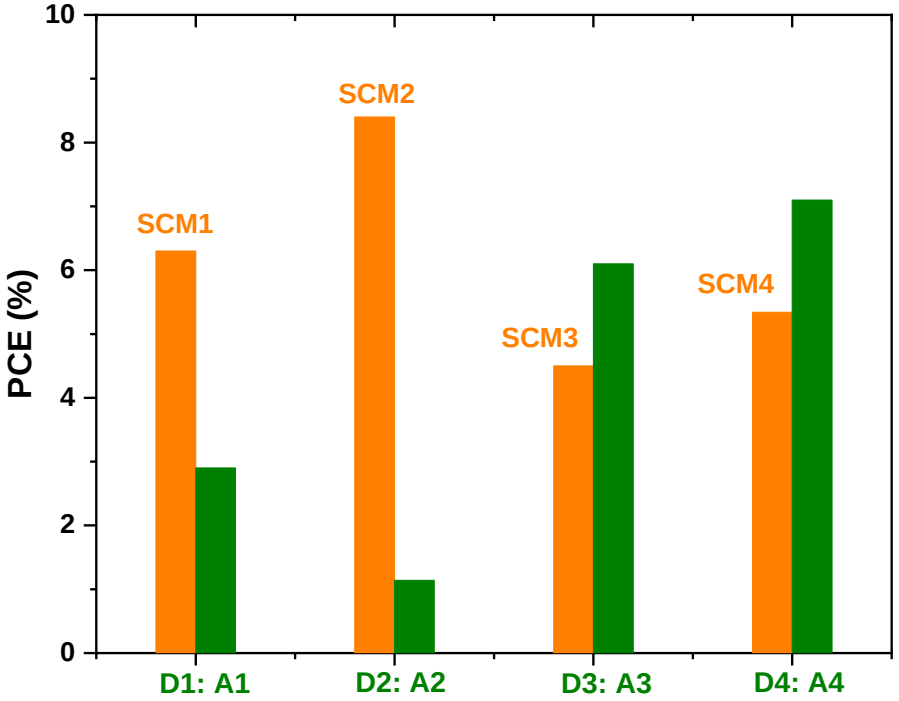




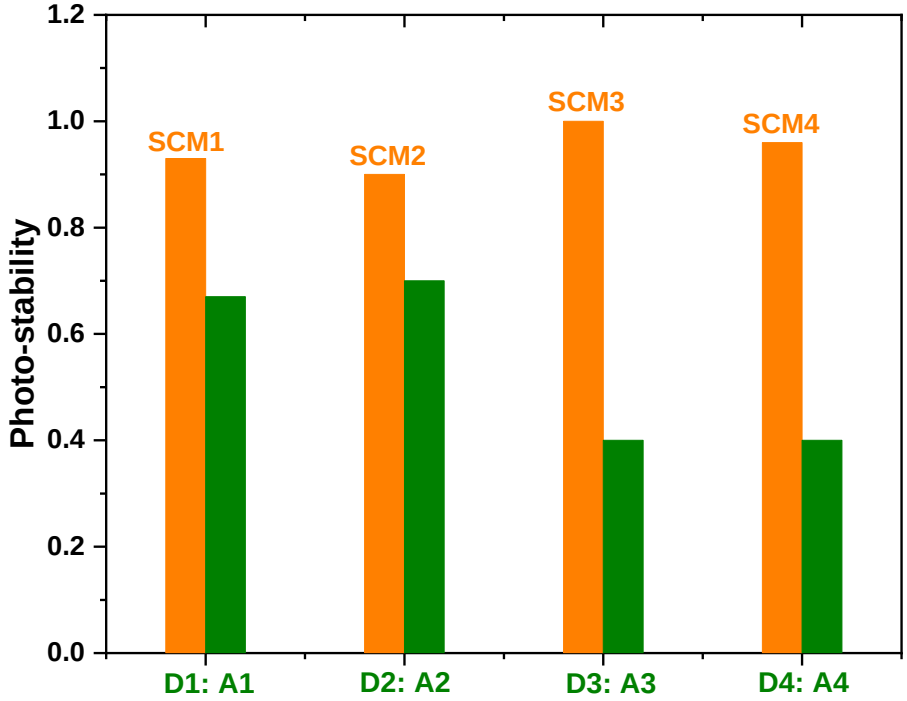
SCM3 is stable under concentrated light.

Y.K. He, N. Li, C.J. Brabec et al. Joule 2022

PCE & Stability

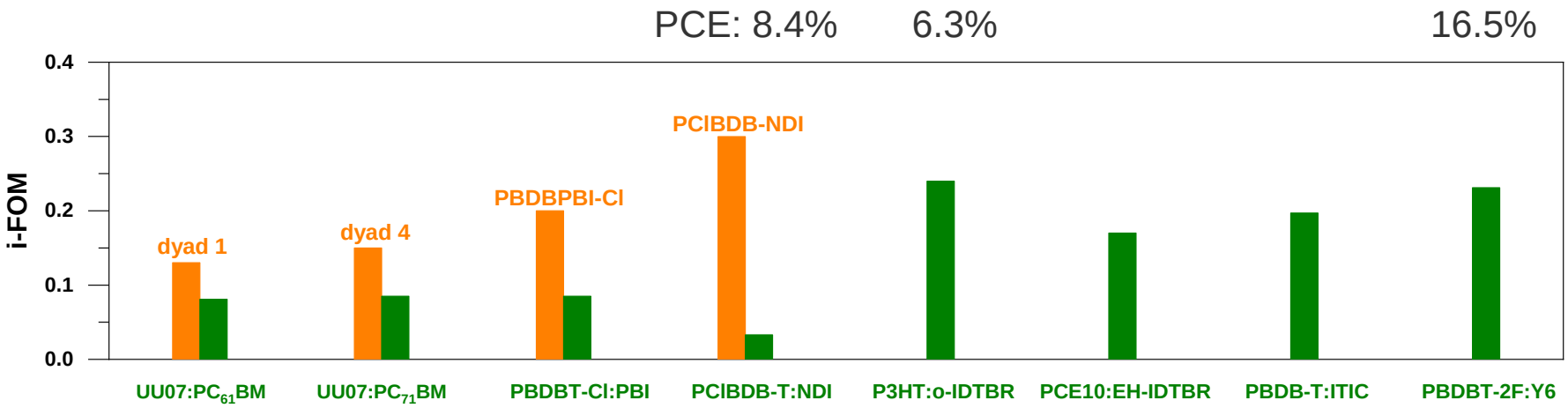


SCMs show higher or comparable PCE with the corresponding BHJs



SCMs show generally enhanced stability than the corresponding BHJs

Industrial figure of merit (i-FoM)



- SCMs exhibit generally higher i-FoM values than their BHJ counterparts.

- PCE does not necessarily decide the final i-FoM.
- All three parameters should be considered.

Y.K. He, N. Li, C.J. Brabec et al. Joule 2022

Acknowledgement

Prof. Christoph J. Brabec
Dr. Ning Li
Erlangen Colleagues

Prof. Peter Bäuerle (Ulm)
Dr. Sebastian Lucas
Anna Aubele

Prof. Weiwei Li (ICCAS)
Dr. Wenbin Lai
Dr. Guitao Feng

Ac

Pro

Dr.

Erla

Thank You