High performance OPV and their applicaton in wearable devices

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Outline

The Status and Challenges of OPV

CH series of high performance OPV materials

Wearable OPV devices

The OPV status

PCE: ~ 20%, still significantly behind of that of inorganic ones

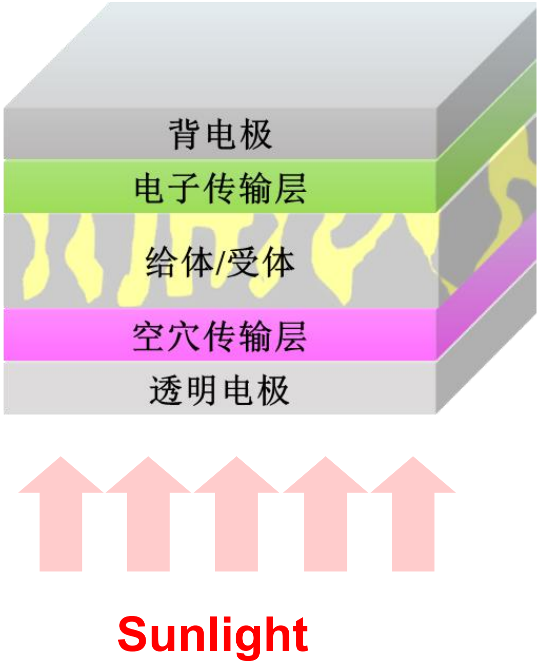
Stability issue

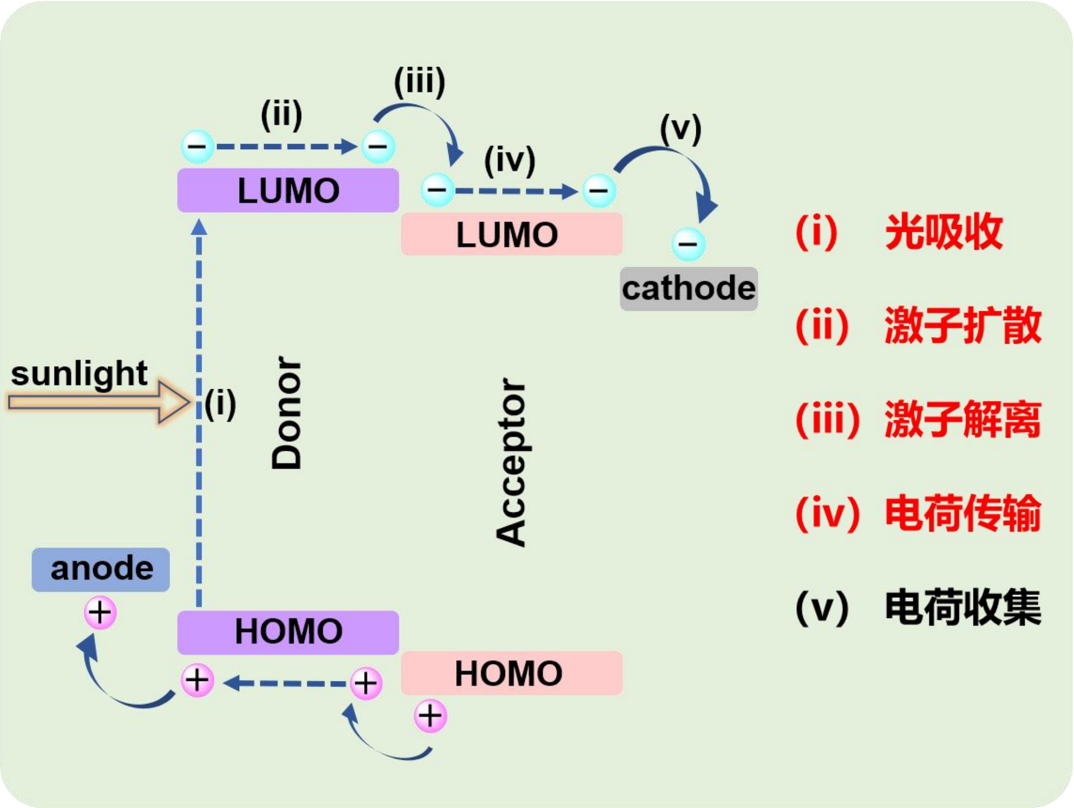
Application cases or where/what to use them?

Current issue for OPV

Materials in the active layer！

The issue：large binding energy leads to large Eloss!



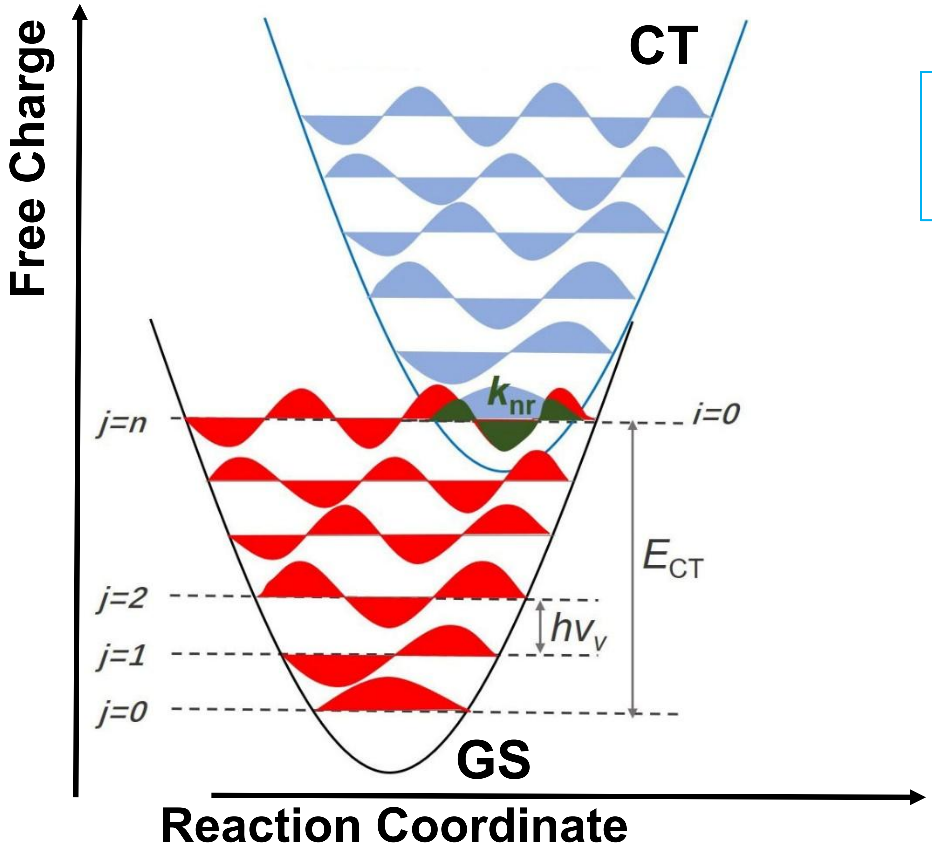


□ Most important process/steps happen at the interface!

Why for the large OPV Eloss?

Reason for large Eloss: serve no-radiatve loss

Mulliken–Hush Model



J. Am. Chem. Soc. 1952, *74*, 811.
Electrochim. Acta 1968, *13*, 1005.

How to reduce： E_{loss}

OPV	Si/PVK
Frenkel Exciton	Wannier Exciton

- **no-radiative loss**

  GaAs/Si ~ 0.04 eV

  OPV > 0.16 eV

- **Material optimization**

  for reduced Krn !

All matters:

- **ground/excited/CT states**
- **Intermolecular interaction**
- **packing, morphology, etc**

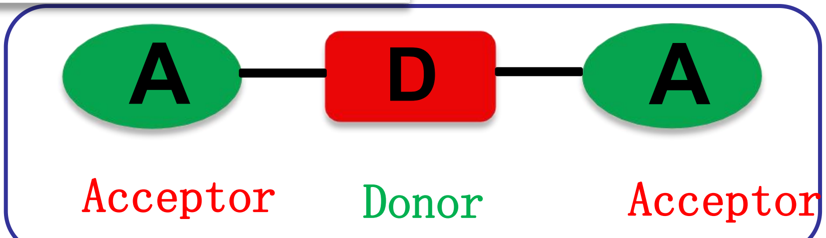
Some of our earlier works

High performance A-D-A molecules !

defined structures/molecules

Polymer

Small mol



Conjugated polymers

+

Small molecules

A-D-A type oligomer like materials

Nature Electronics, *2019*, 2, 513
Science 2018, 361, 109
Nature. Photon. 2017, 11, 85
Nature Photon., 2015, 9, 35
Acc. Chem. Res., 2013, *46*, 2645

***Adv. Mater*, 2019**,1804723
***Adv. Mater*, 2018**, 30, 1707508
J. Am. Chem. Soc, **2015**, *137*, 3886
J. Am. Chem. Soc, **2014**, 136, 15529
J. Am. Chem. Soc., **2013**, *135*, 8484
J. Am. Chem. Soc., **2013**, *135*, 5921
J. Am. Chem. Soc., **2012**, *134*, 16345
J. Am. Chem. Soc., **2013**, *135*, 5921

A semi-empirical model for OPV

SQ （Shockley-Queisser）PV model，Alan Heeger OPV model

A semi-empirical model for OPV

$$V_{oc} = \frac{1}{q}(E_g - E_{loss}) = \frac{1}{q}(\frac{1240}{\lambda} - E_{loss})$$

$$J_{sc} = \int_{300}^{\lambda} \frac{q\lambda}{hc} \cdot E(\lambda) \cdot EQE(\lambda) \cdot d\lambda$$

$$PCE(\%) = V_{oc} \cdot J_{sc} \cdot FF/P_{in} = \frac{1}{e}[\left(\frac{1240}{\lambda} - E_{loss}\right) \cdot \int_{300}^{\lambda} \frac{q\lambda}{hc} \cdot E(\lambda) \cdot EQE(\lambda) \cdot d\lambda \cdot FF/P_{in}$$

Based on

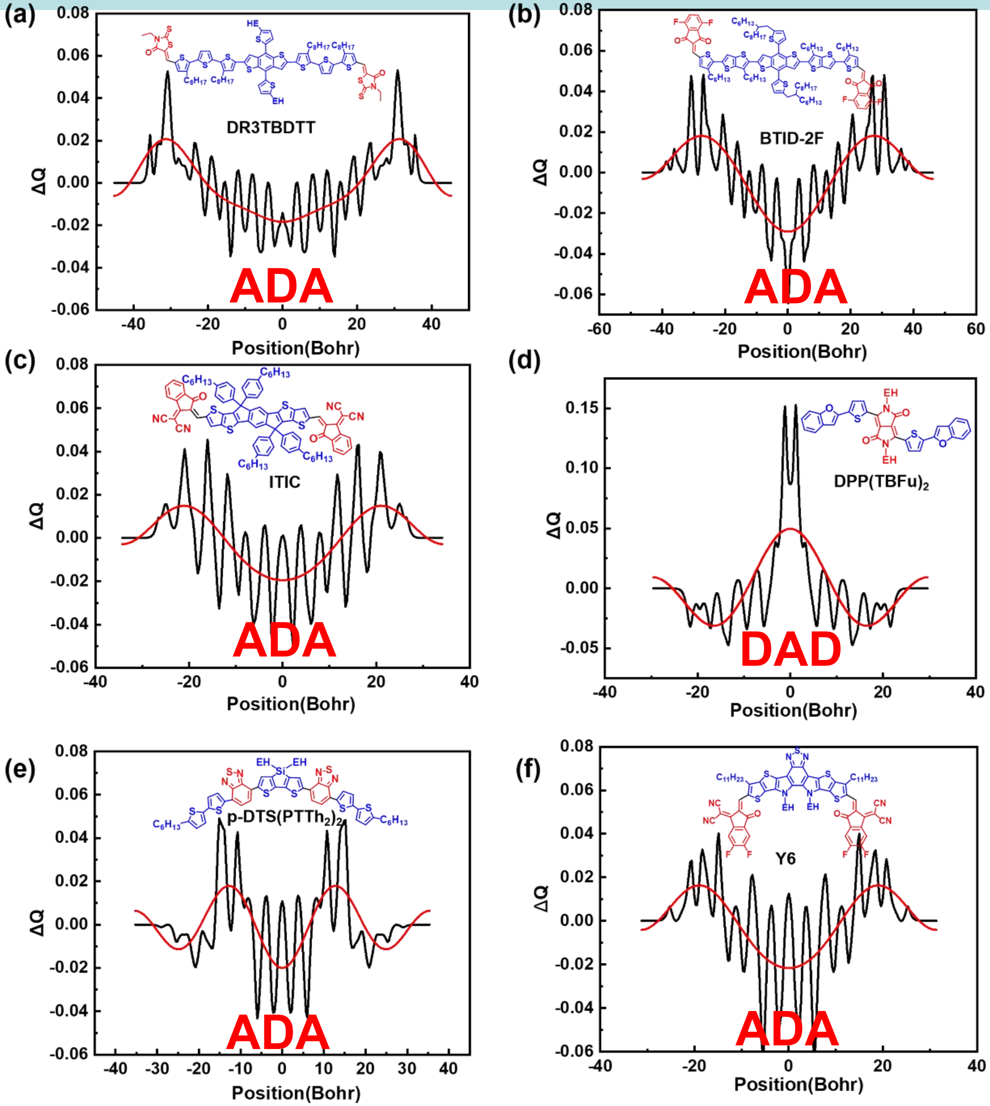
- **Balanced Theory**
- **Shockley-Queisser Limit Theory**
- **(SQ Limit for photovoltaic device)**
- **State-of-the-art experimental results**

A semi-empirical model, for both material design and optimiza

Science 2018, 361, 109; *J. Mater. Chem. A*, 2020, 8, 9726

The characteristics of ADA type compounds

Why ADA molecules are better：A-D-A vs D-A-D



What are ADA molecules (vs DAD)?
most unique characteristics/特征?

HOMO/LOMO
Electron density distribution

$$\Delta Q = \Psi^2_{LUMO} - \Psi^2_{HOMO}$$

Charge density difference between excited state and ground state

U vs reverse T type
frontier electron density distribution

Chem. Soc. Rev. 2020, *49*, 2828.

The characteristics of ADA materials

Why A-D-A is better than DAD etc?

Unique and optimal
spatial electron distribution at front (excited) orbitals

1) Facilitated exciton dissociation
2) Optimized Morphology for charge transportation
3) Stable and 2D/3D networked packing
4) Smaller Eloss

How we can get better?

Chem. Soc. Rev. 2020, *49*, 2828.

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CH series of high performance OPV materials

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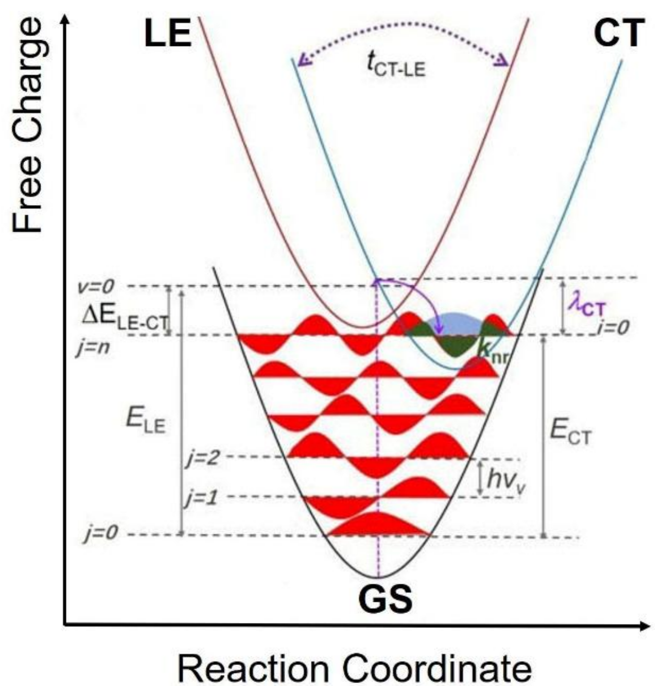
Charactristics of CH Series OPV molecules

2D conjugation extention for smaller reorganization energy and higher FL molecules

非富勒烯体系“三态” 模型

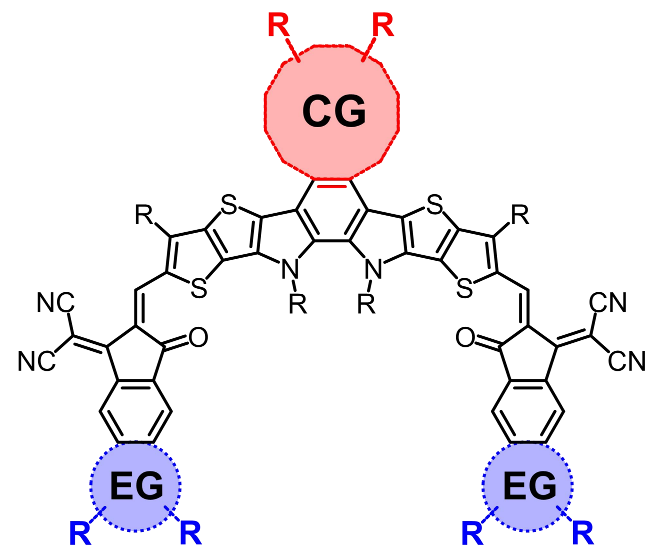


Nat. Energy 2021, *6*, 799.

☞2D conjugation
☞Rigid structure

→

☞Reduce reorganization energy
☞Reduce excion bonding energy
☞Strength π-π packing

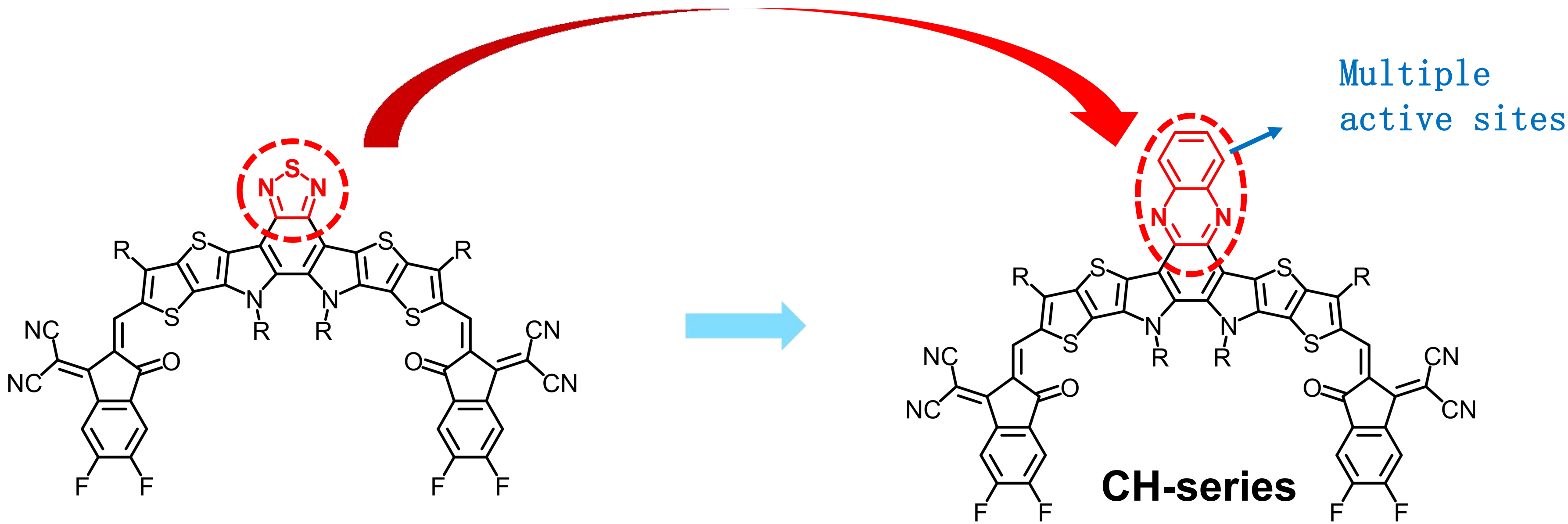


Get better molecules:

- ☐ **High flurescence**
- ☐ **Increase CT state**
- ☐ **Reduce the coupling between CT & GS**

Some examples of CH series materials

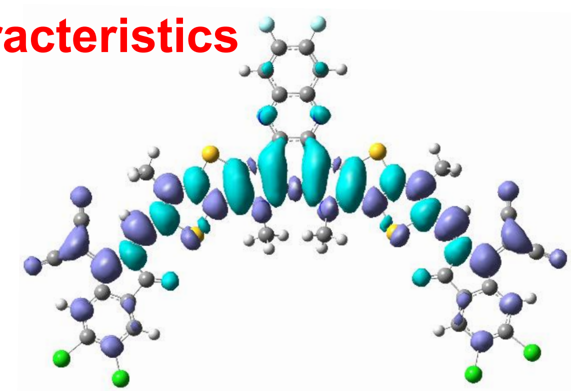
1. Central unit conjugation extension



Advantages:

- smaller reorganization energy
- stronger intermol packing
- Optimze packing modes
- Better potential for optimization

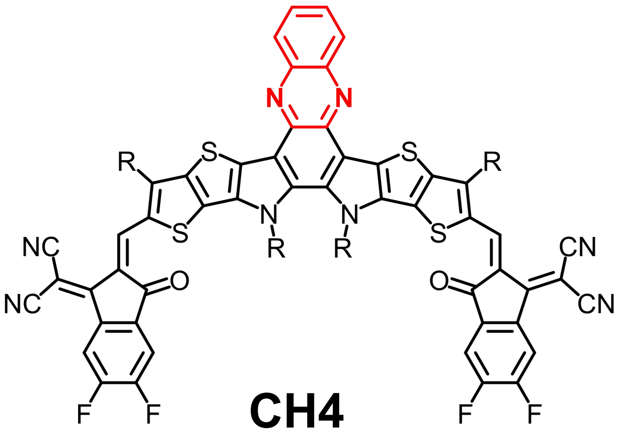
A-D-A characteristics

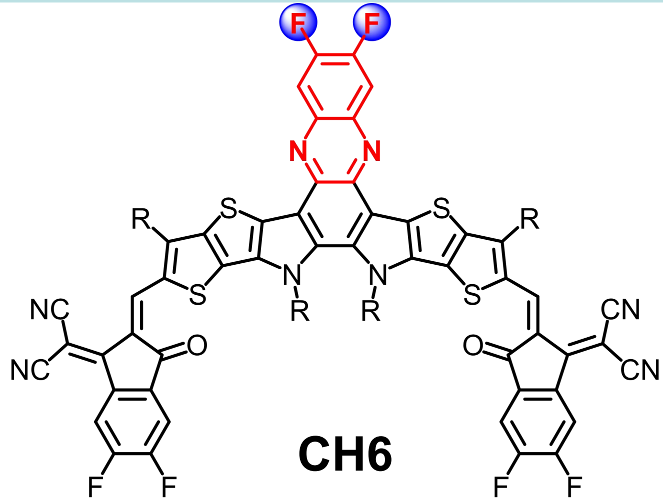


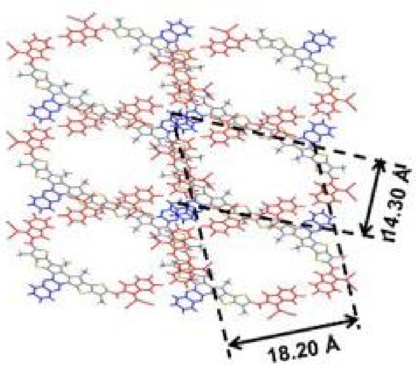
$$\Delta Q = \Psi^2_{LUMO} - \Psi^2_{HOMO}$$

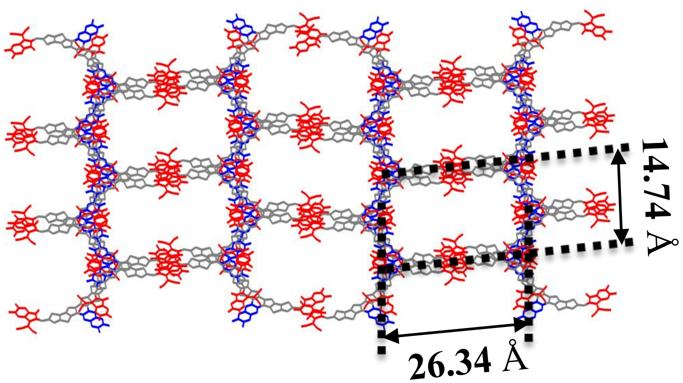
CH series of ADA type high performance molecules

2. F-subsitituted central unit









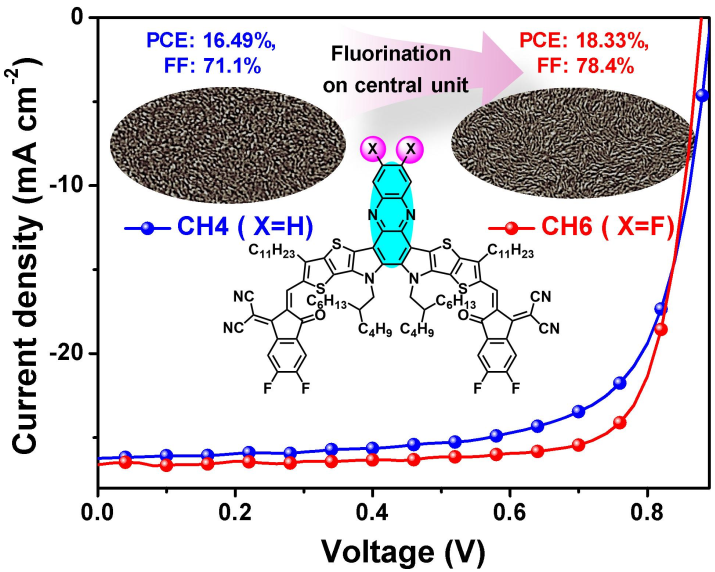
- Optimized packing due to the F-end group
- Stronger and more packing from the central unit

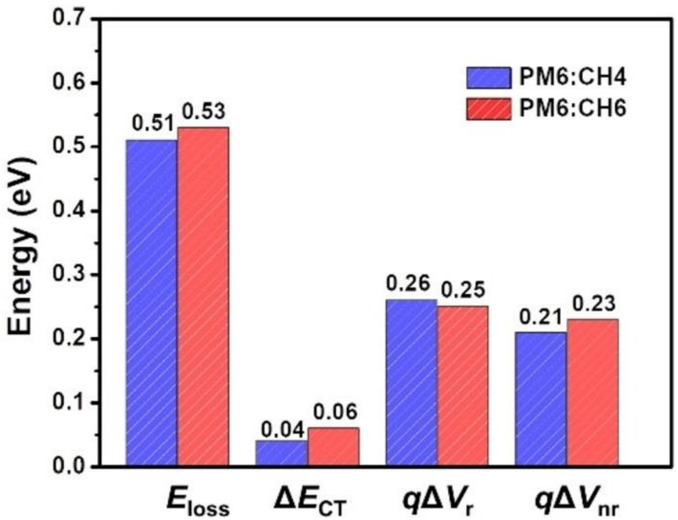
- The packing mode from the central unit

Angew. Chem. Int. Ed. 2022, 61, e202209580.

CH series of ADA type high performance molecules

F-subsititution leads to better performance



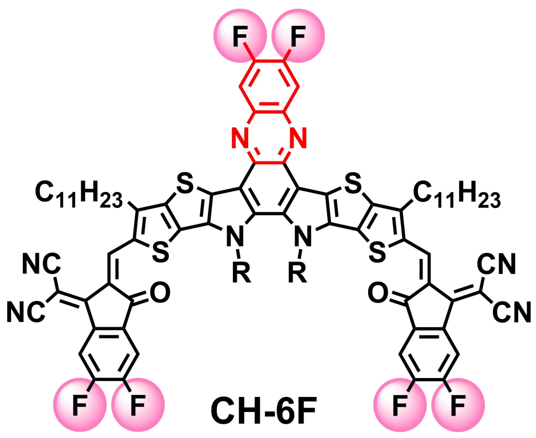


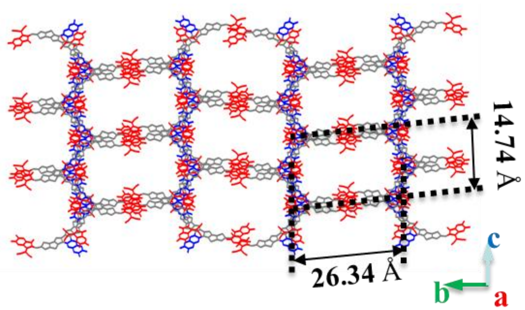
- ☐ Better morpholohy and higher PCE（18.33% vs 16.49%）
- ☐ Smaller Eloss

Angew. Chem. Int. Ed. 2022, 61, e202209580.

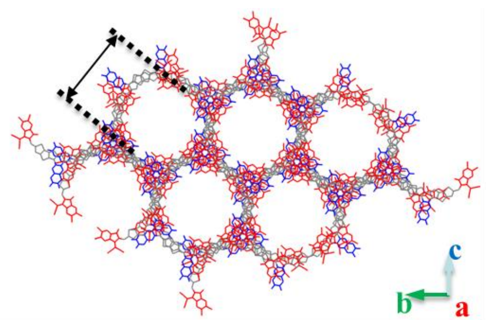
CH series of ADA type high performance molecules

3. More peripheral X subsititation: 18.22% PCE

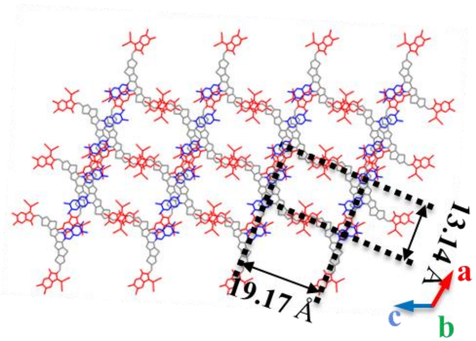




CH-6F monoclinic system



CH-4Cl trigonal system



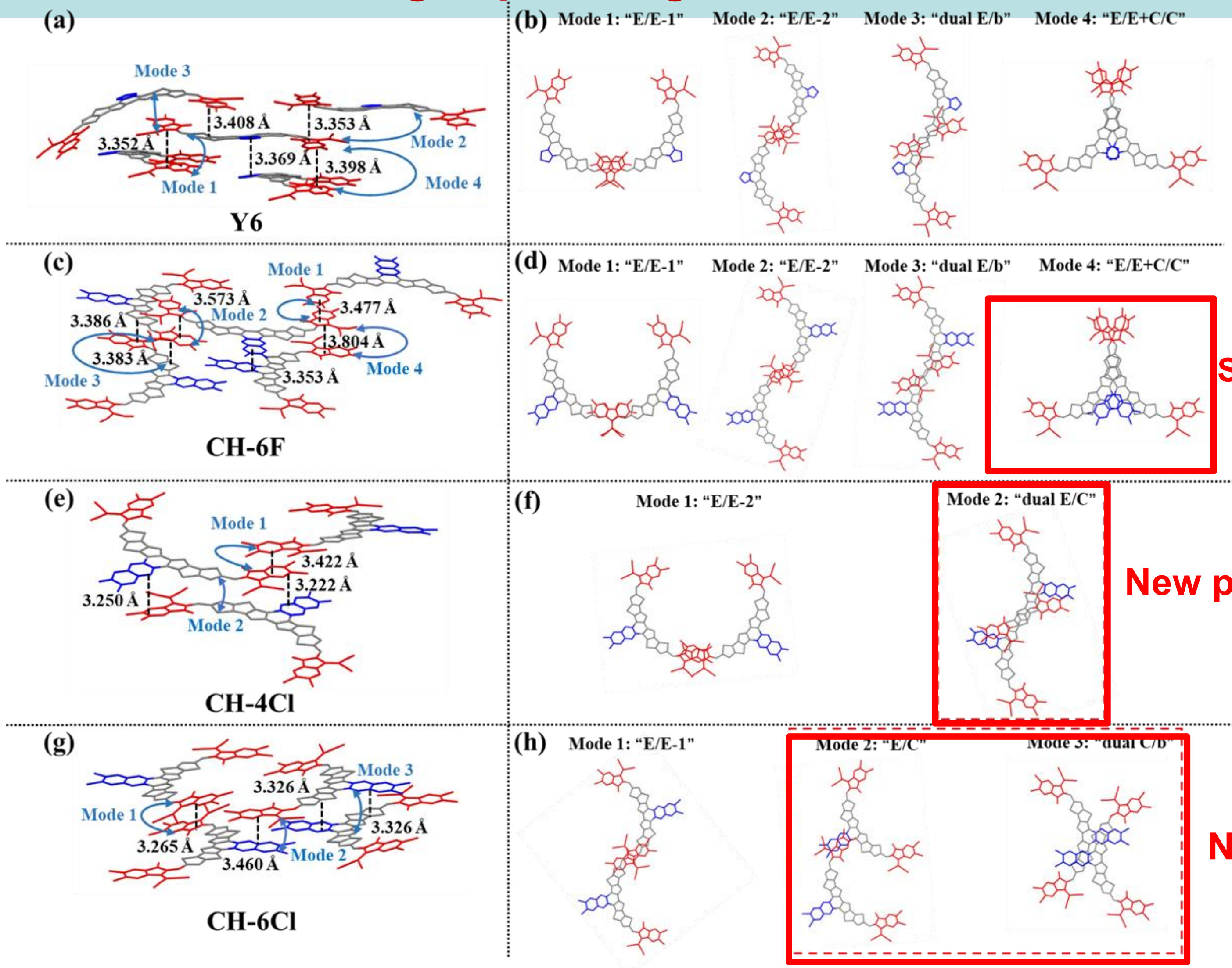
CH-6Cl triclinic system

☐ Fine tuning of X → ☐ Packing changed singnificantly

Energy Environ. Sci. 2022, *15*, 3519
Angew. Chem. Int. Ed., 2023, *61*, e202312630.

CH series of ADA type high performance molecules

New and stronger packing mode > Smaller Eloss



Stronger packing

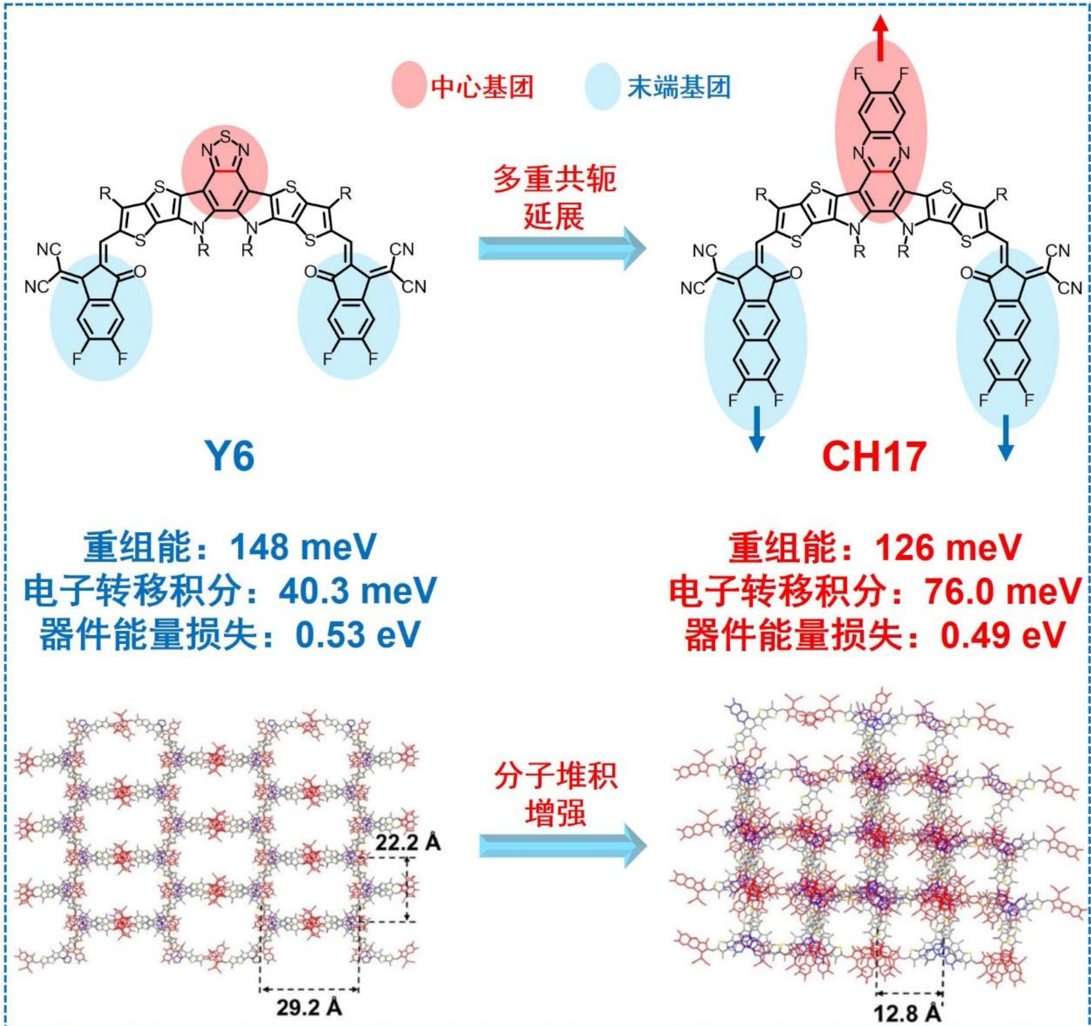
New packing mode

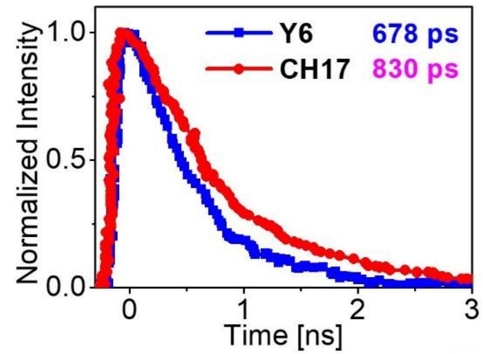
New Packing m

Energy Environ. Sci. 2022, *15*, 3519.

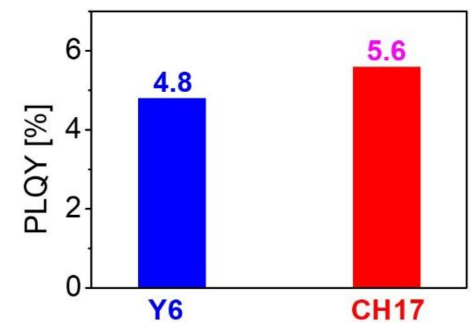
CH series of ADA type high performance molecules

4. Mutiple conjugation extention





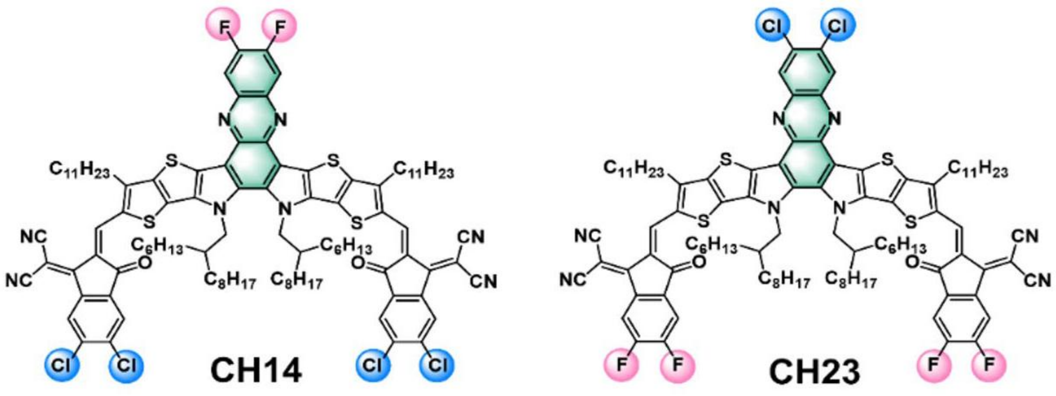
更小重组能
更长激子寿命
更高荧光量子产率
更低器件能量损失

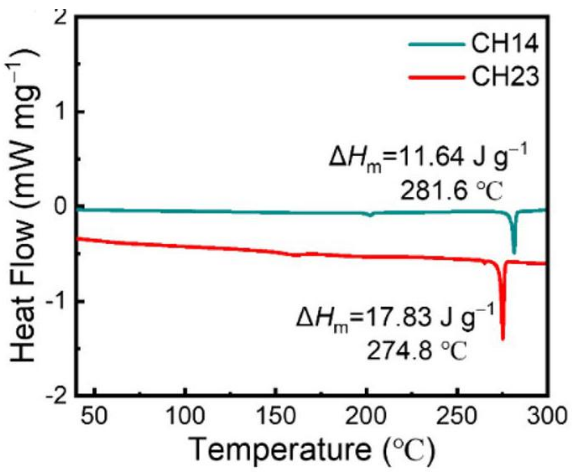


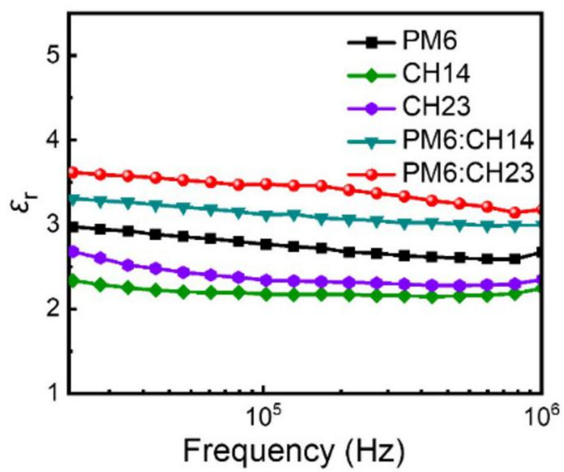
Sci. China Chem. 2022, *65*, 1362.

CH series of ADA type high performance molecules

5. Dielectric consistant turning







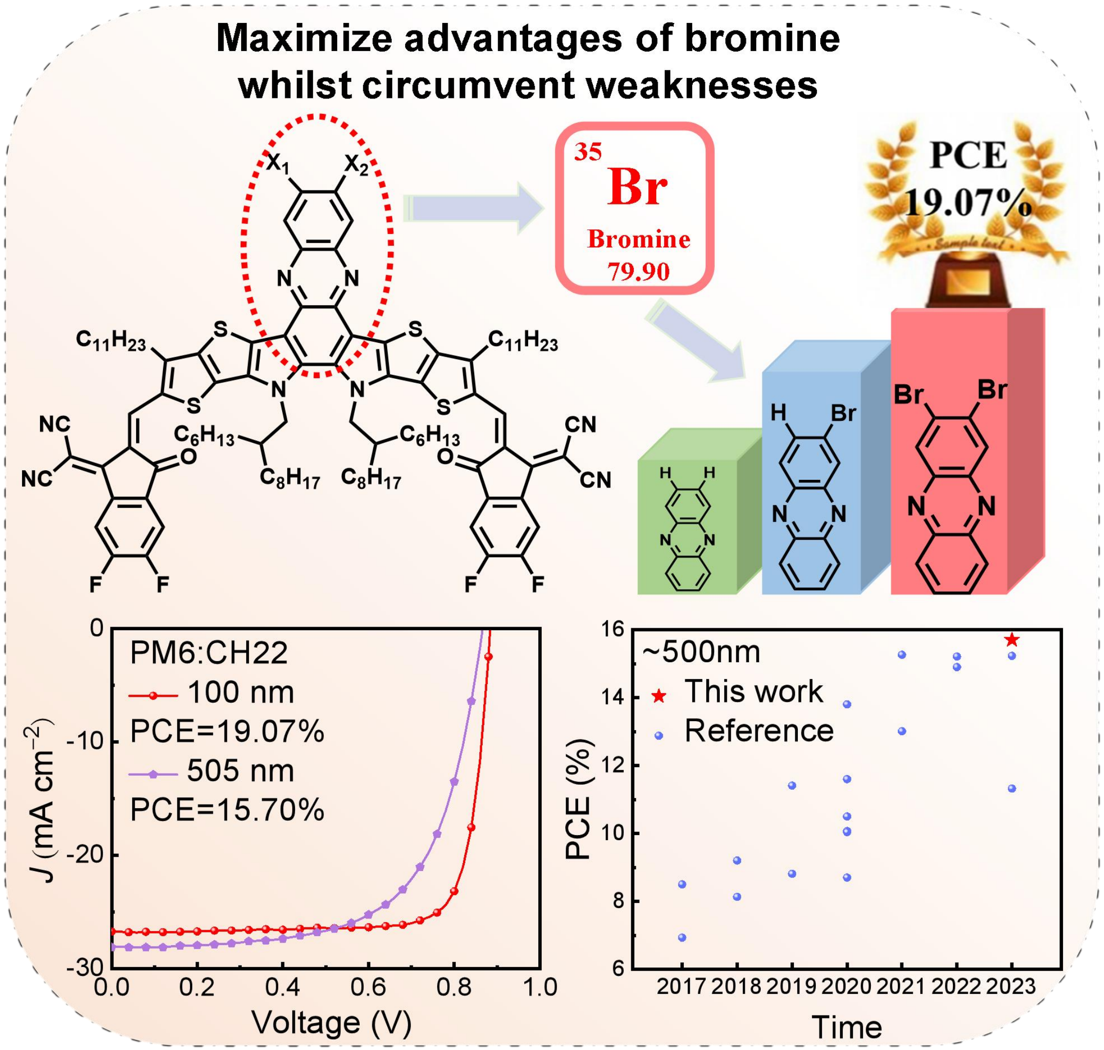
- CH23 higher packing density
- Enhanced charge transfer
- 18.77% PCE of binary device

larger dielectric constant due to enhance packing & halogen subsitition

Adv. Funct. Mater. 2023, 2301573

CH series of ADA type high performance molecules

Bromided CH material for PCE > 19%



Br atom and related molecules

- Easier polerization, better crystalline
- Larger steric hindance
- Optimized approach: introduce Br at the central unit

- Stronger and more ordered packing
- Larger Ɛ、Smaller E of binding
- PCE of 19.06% for binary device
- 500 nm thickness device with 15.7%PCE

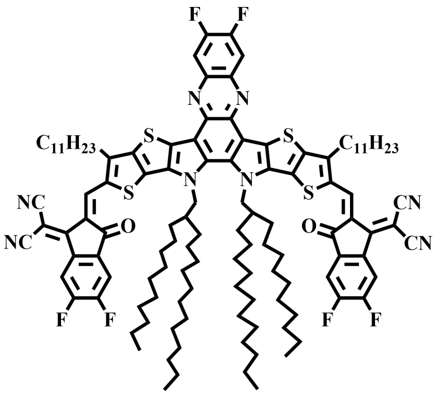
A race of for brmoide materials

Nature Communications | (2023) 14:4707

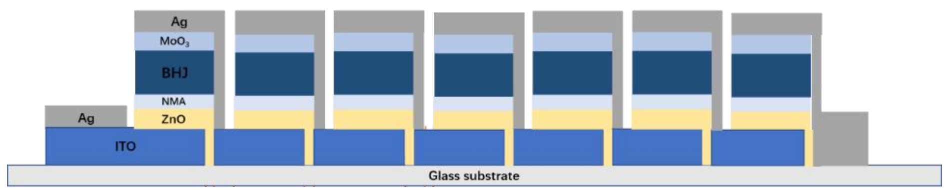
CH series of ADA type high performance molecules

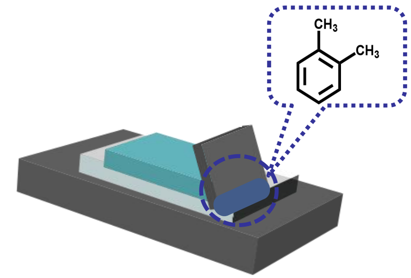
6. OPV module

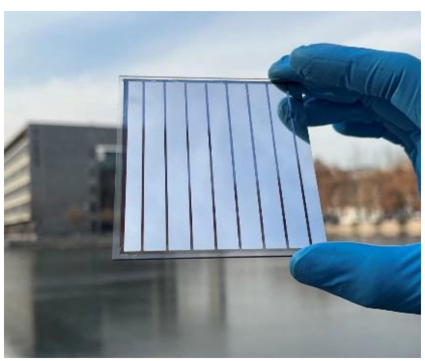
- Blade coating for large OPV module (25 cm^2)
- PCE of 14.42%，92% remains after 500 h under MPP

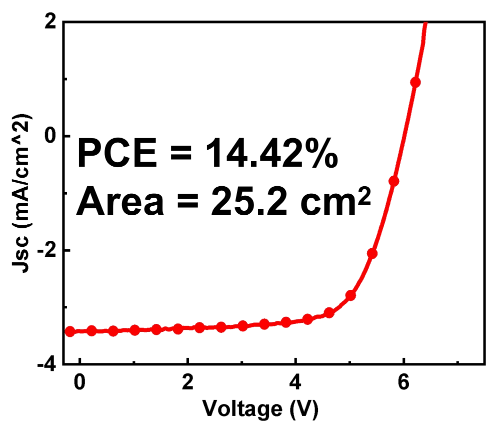


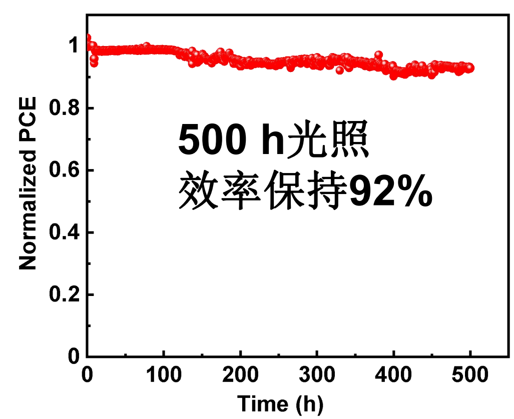
CH7







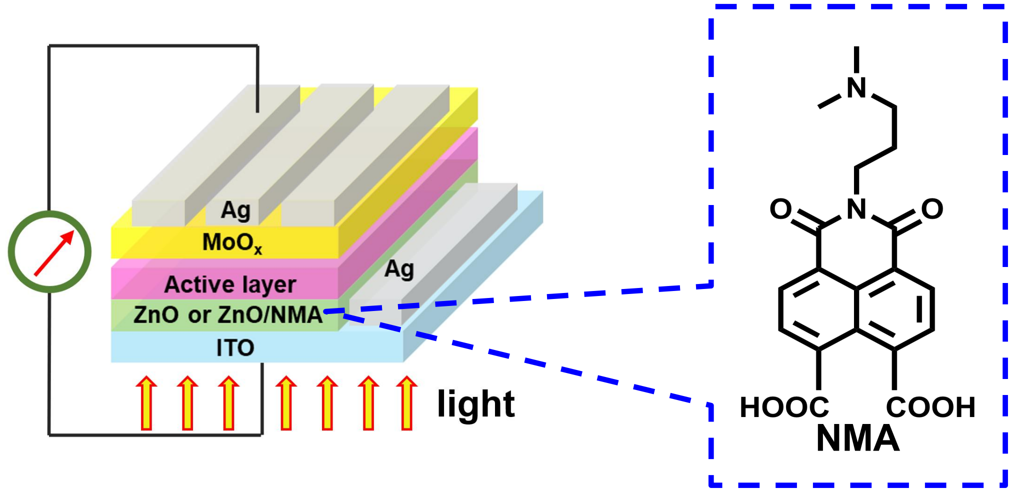


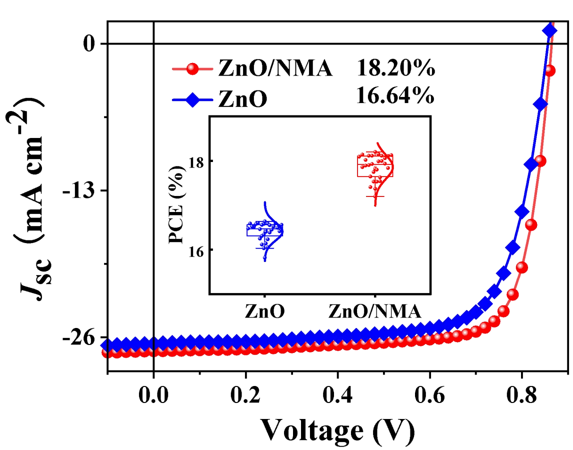


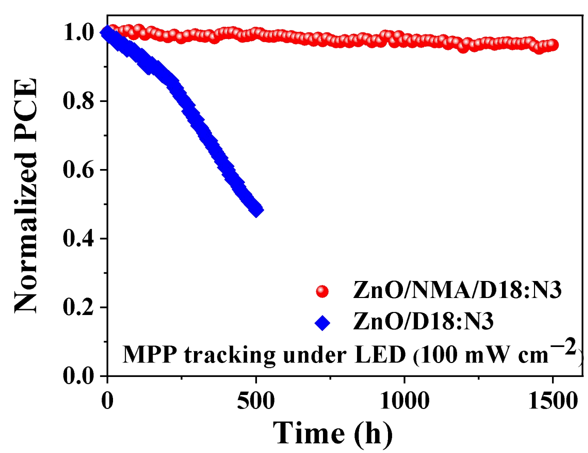
Solar RRL 2023, 7, 2300029

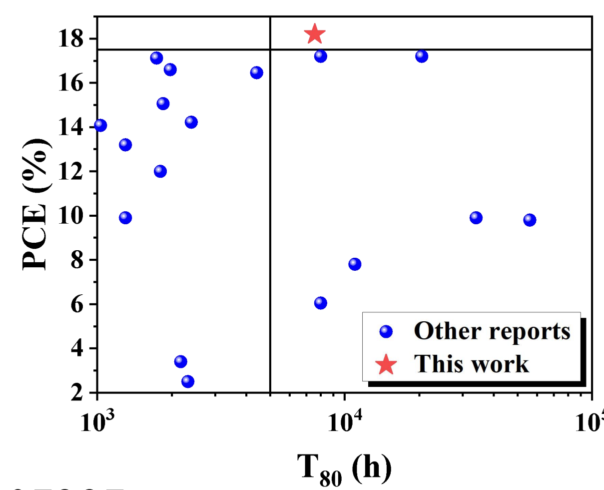
Both stable and high performance OPV

- **HTL NMA—High reverse OPV with high performance**
- **Life time > 5 years—The best stability with PCE > 18% under MPP conditions**







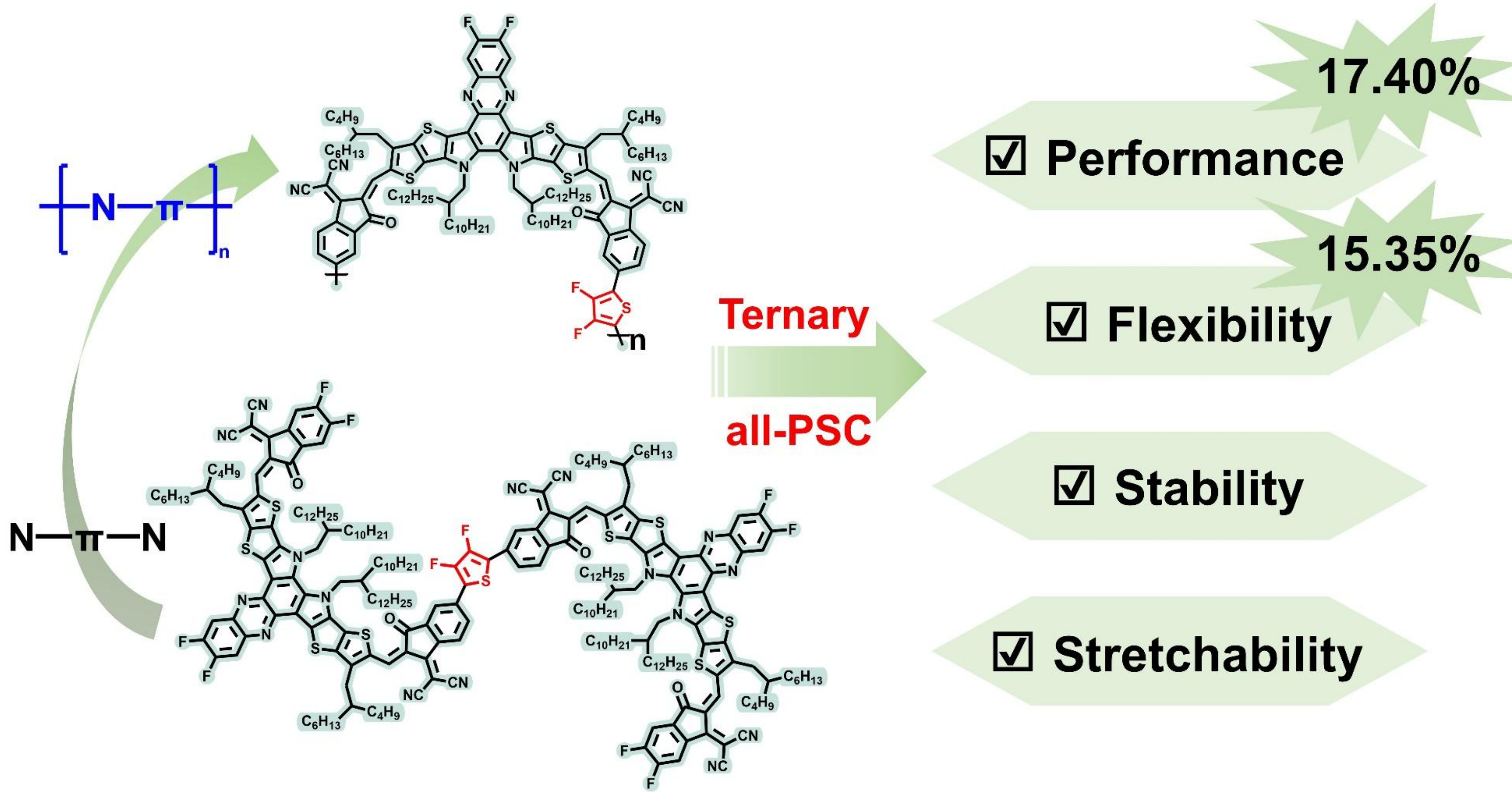


Angew. Chem. Int. Ed., **2022**, e202207397

Dimer of CH acceptor materials

CH series of ADA type high performance molecules

7. Dimers of CH series materials



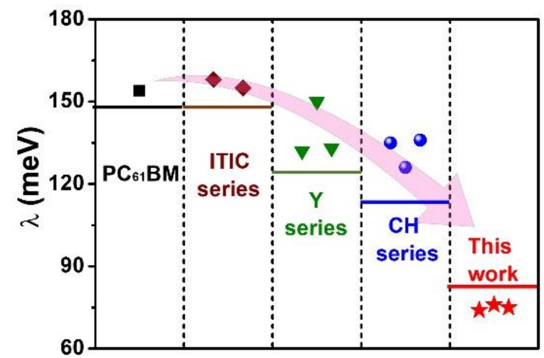
Adv. Energy Mater. 2023, DOI: 10.1002/aenm.202300301.

CH series of ADA type high performance molecules

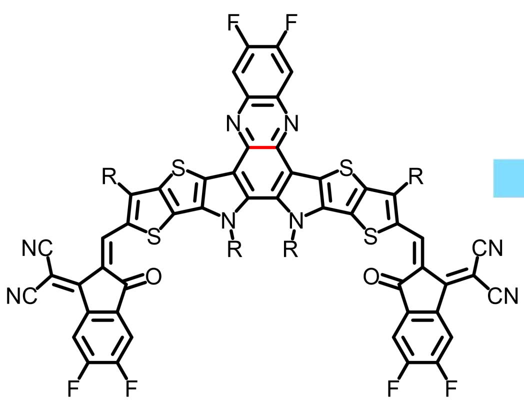
8. Dimers of CH molecules connected at the central unit

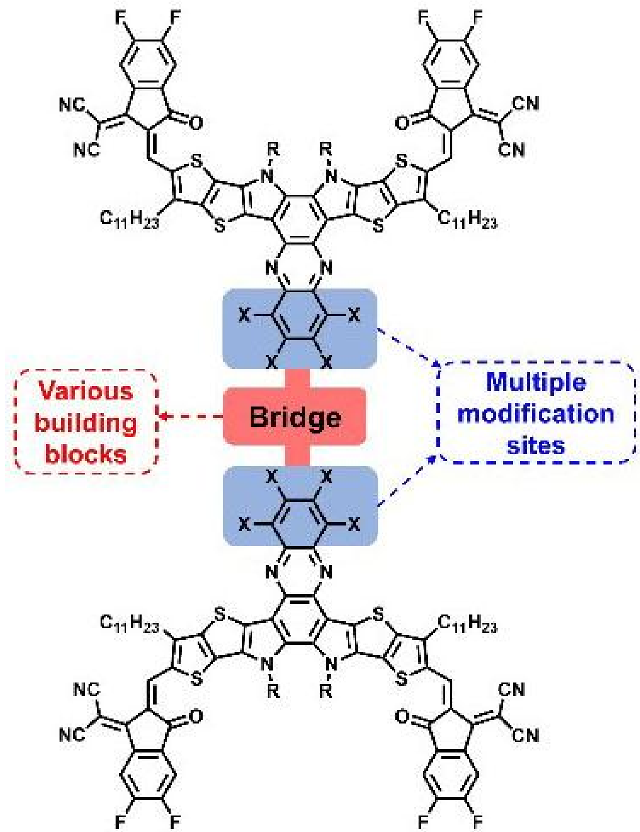
3D acceptors with multiple CH A–D–A units

Reduced reorganization energy



Monomer to Dimer

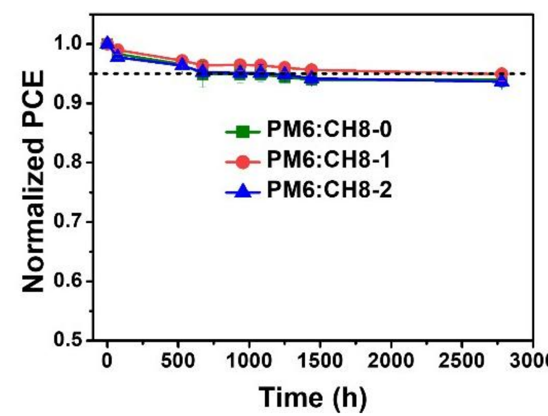




- Novel dimerzation
- Avoid interfered end packing

T_g increased and remained end packing

- PCE > 17%
- Enhanced stability

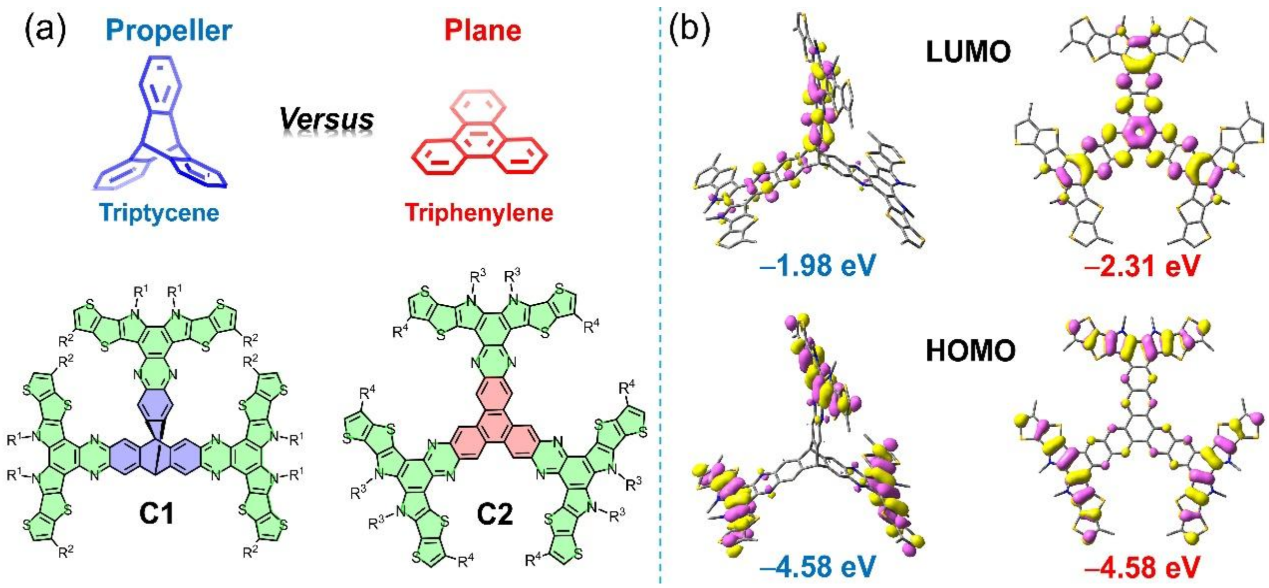


Energy Environ. Sci. 2023, 16, 1773

Angew. Chem. Int. Ed., 2023, e202307962

CH series of ADA type high performance molecules

planar vs propeller type molecules



CH25 **CH26**

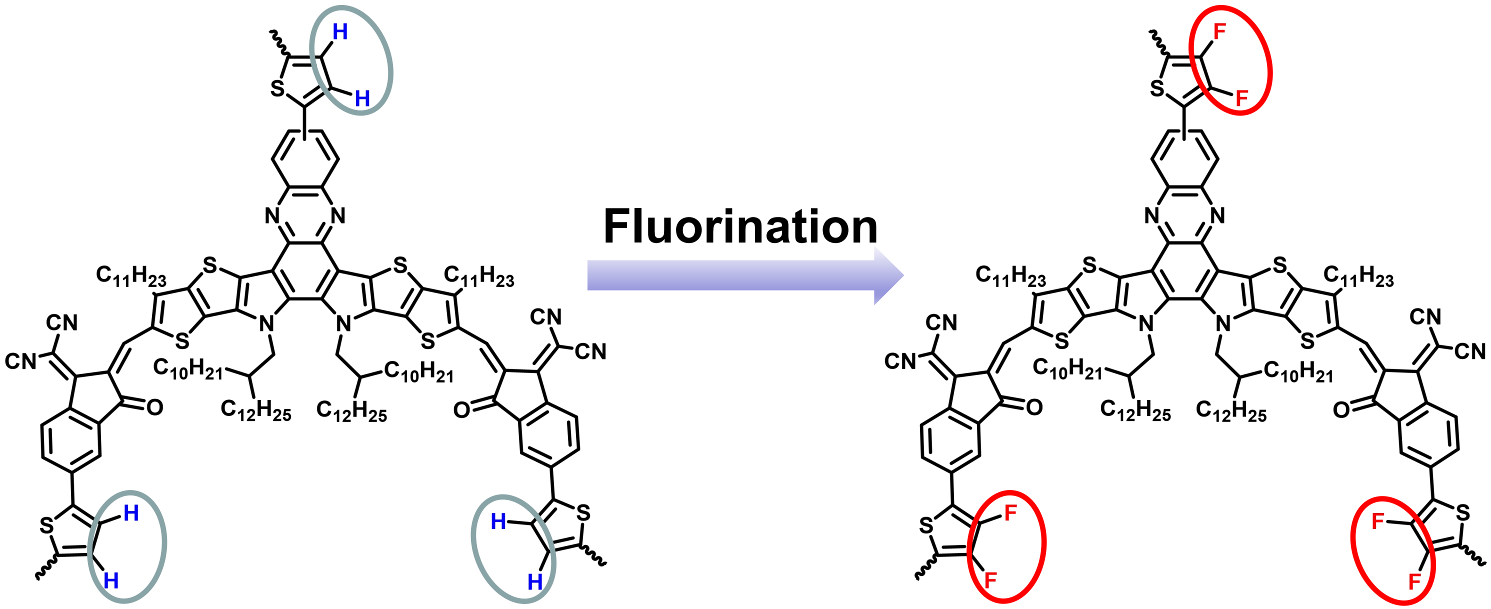
Active Layers	V_{OC} [V]	J_{SC} [mA cm^{-2}]	Calc. J_{SC}[b] [mA cm^{-2}]	FF [%]	PCE [%]
PM6:CH25	0.840 (0.836±0.010)	4.82 (4.19±0.35)	4.33	55.4 (55.4±0.8)	2.24 (1.91±0.19)
PM6:CH26	0.920 (0.922±0.003)	22.98 (22.60±0.22)	22.49	72.7 (77.3±0.4)	15.41 (15.11±0.17)

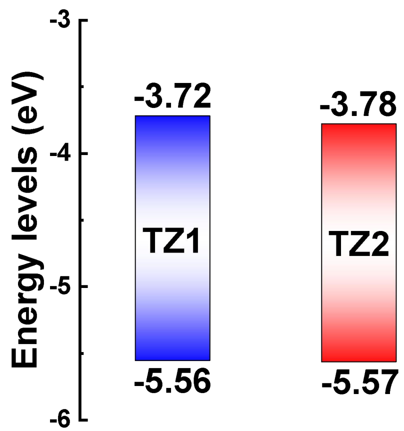
Angew. Chem. Int. Ed., 2023, 62, e202311686

Polymerized CH acceptor materials

CH series of ADA type high performance molecules

9. Polymerized CH type molecules



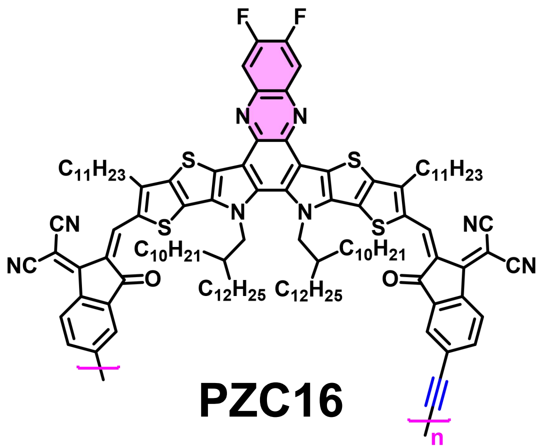


- 3D conjugation extension
- All-polymer device with PCE of 7.41%

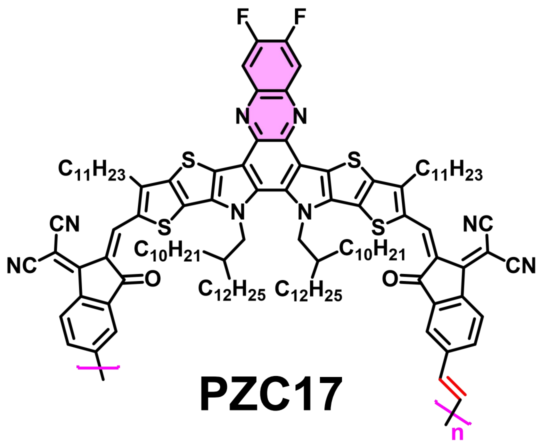
Org. Electron. 2023, *114*, 106735.

CH series of ADA type high performance molecules

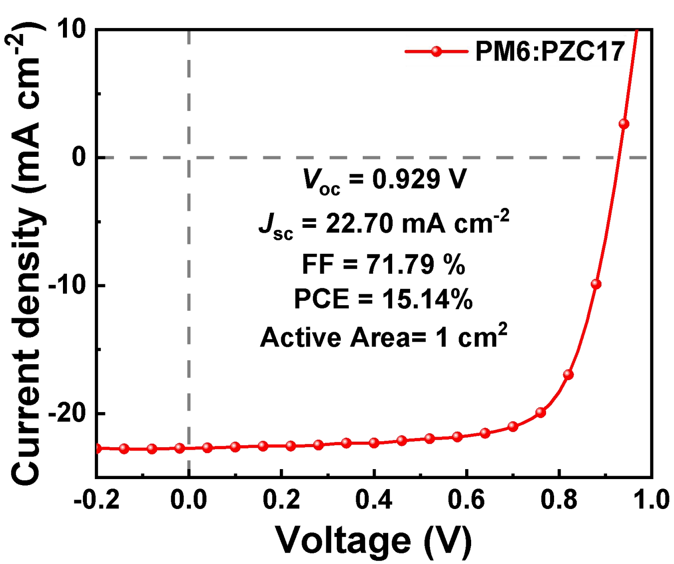
Different linker: double vs triple CC bonds



PZC16



PZC17

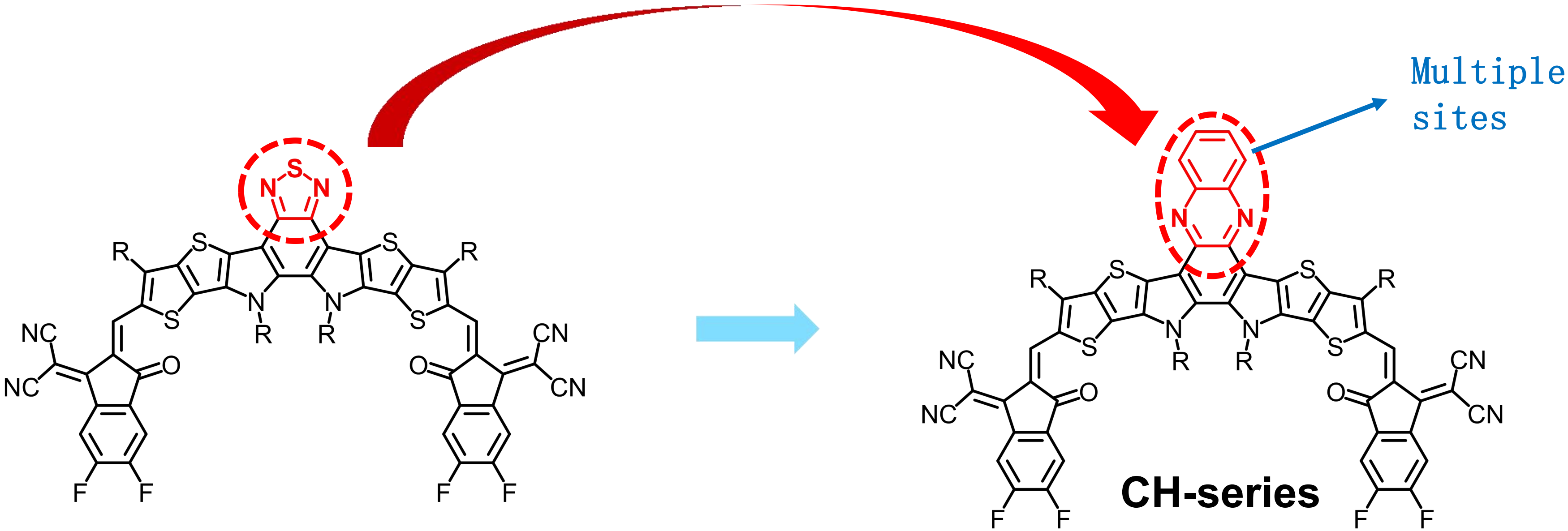


- Double/triple bond enhance ordered packing
- PCE of 16.33 for binary PM6:PZC17 device
- 15.14% PCE for 1cm^2 device

Adv. Funct. Mater. 2023, 2214248.

CH series of ADA type high performance molecules

Short summary: CH is a great platform for multiple optimization



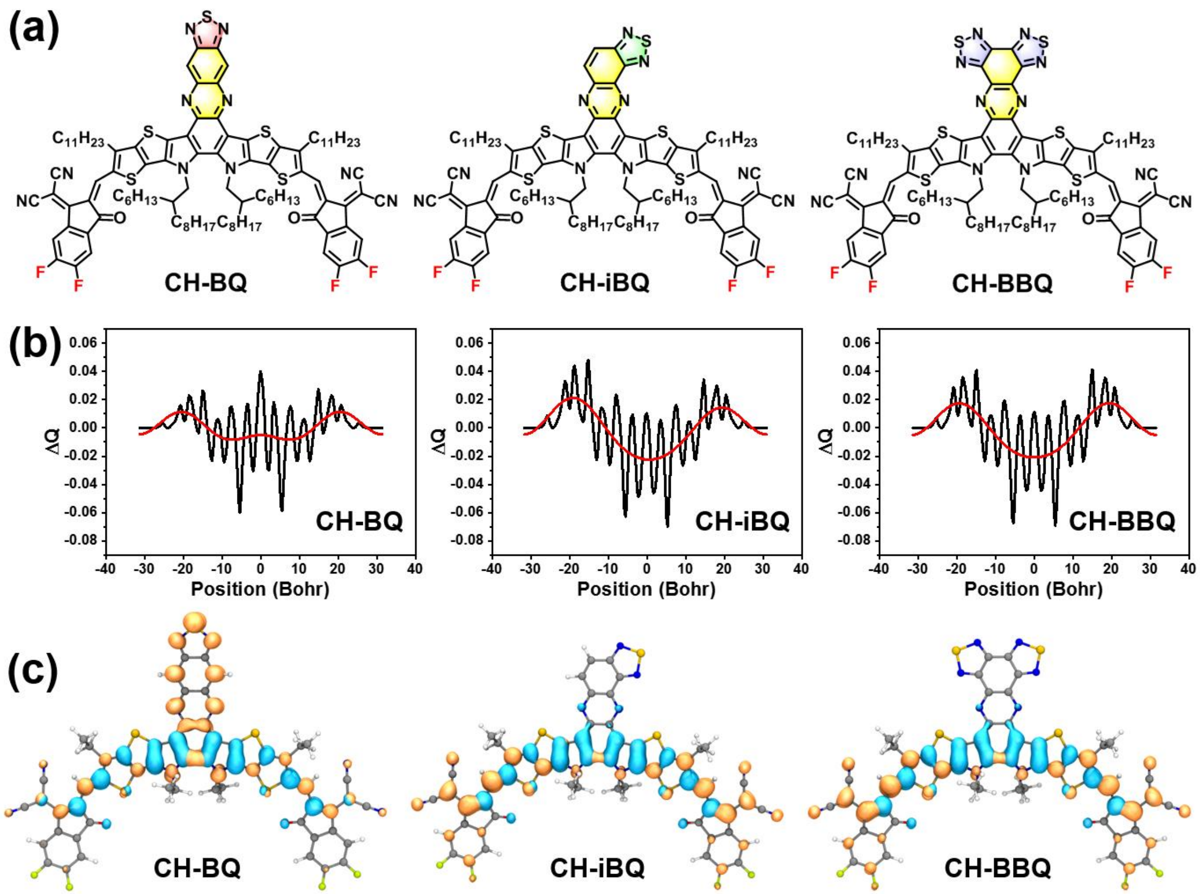
More diverised and optimization in terms of molecular design!

Single molecules, oligomers and polymers

More structure optimization = Better PCE imporvement possibility

CH series of ADA type high performance molecules

Mutiple conjugation extension



PCE ~ 19%

Angew. Chem. Int. Ed., 2023, e202308832

Ontline

The Status and Challenges of OPV

CH series of high performance OPV materials

Wearable OPV devices

Where are OPV for?

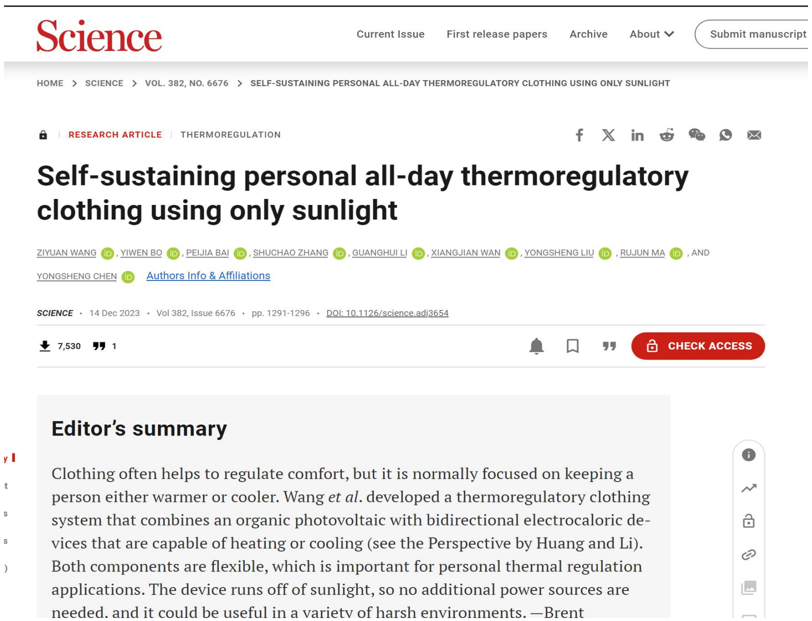
轻，薄，柔，透光

Light, thin, flexibe, transparent

Weable OPV and its applications

Solar-powered clothes, for the heat and cold

Flexible OPV-EC thermoregulatory clothing (OETC):
cooling in sunlight, warming in dark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RESEARCH ARTICLE | THERMOREGULATION

Self-sustaining personal all-day thermoregulatory clothing using only sunlight

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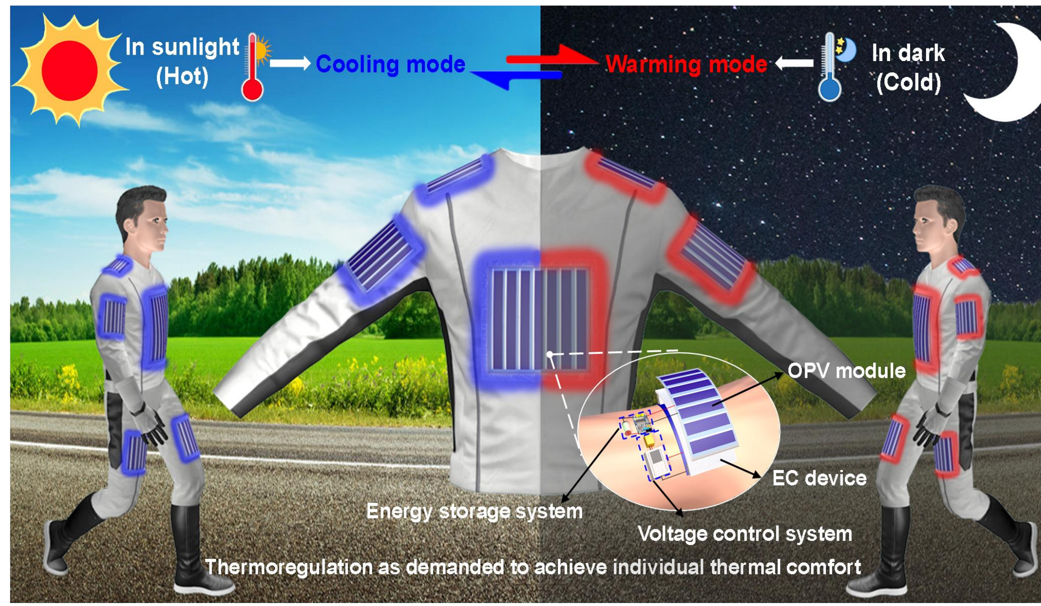
Editor's summary

Clothing often helps to regulate comfort, but it is normally focused on keeping a person either warmer or cooler. Wang *et al*. developed a thermoregulatory clothing system that combines an organic photovoltaic with bidirectional electrocaloric devices that are capable of heating or cooling (see the Perspective by Huang and Li). Both components are flexible, which is important for personal thermal regulation applications. The device runs off of sunlight, so no additional power sources are needed, and it could be useful in a variety of harsh environments. —Brent



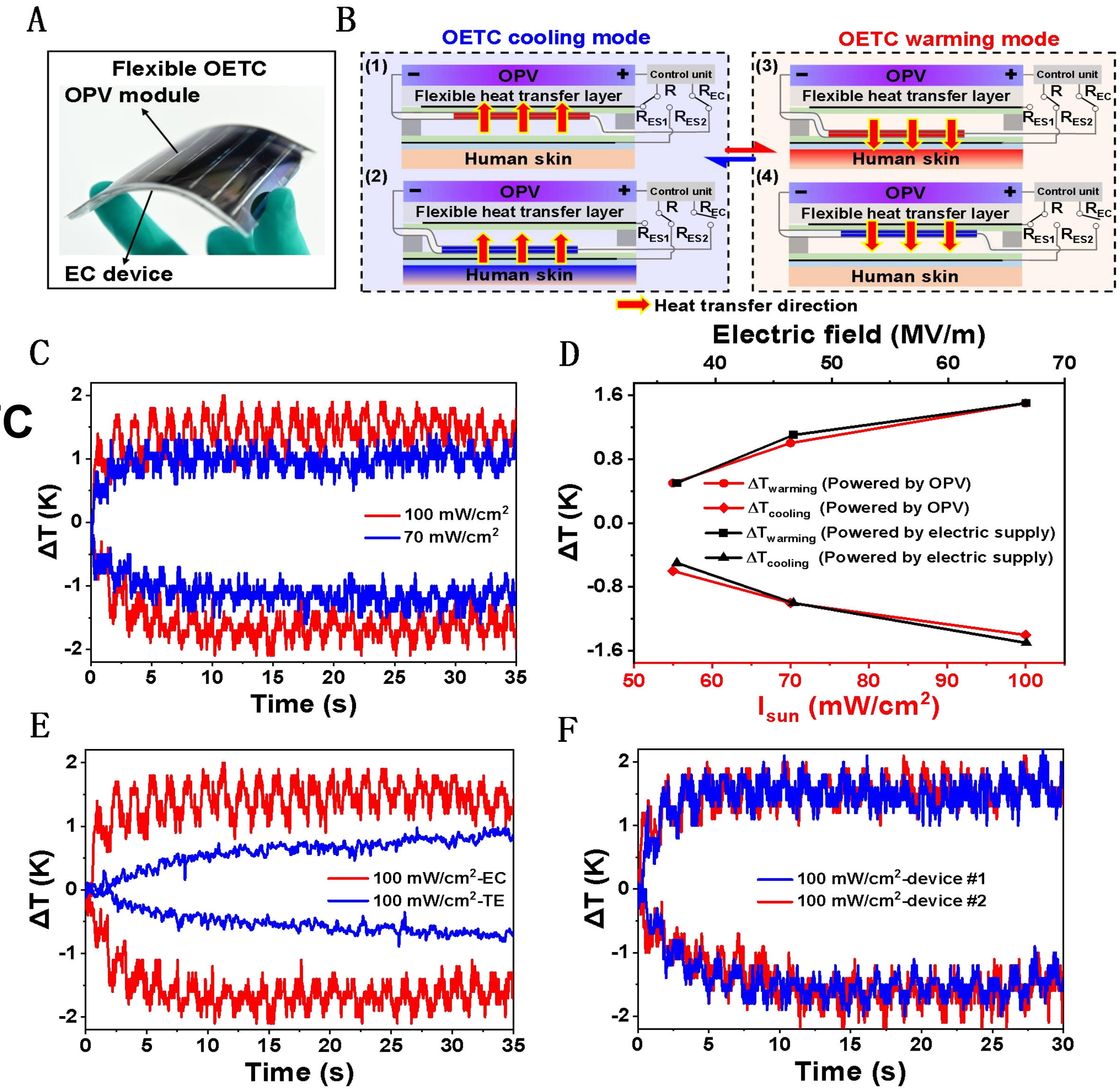
Outdoor, space, polar regions

Z. Wang, R. Ma, Y. Liu, Y. Chen, et al, Science, 2023, 328, 1291-1296

Self-sustaining personal all-day thermoregulatory clothing using only sunlight

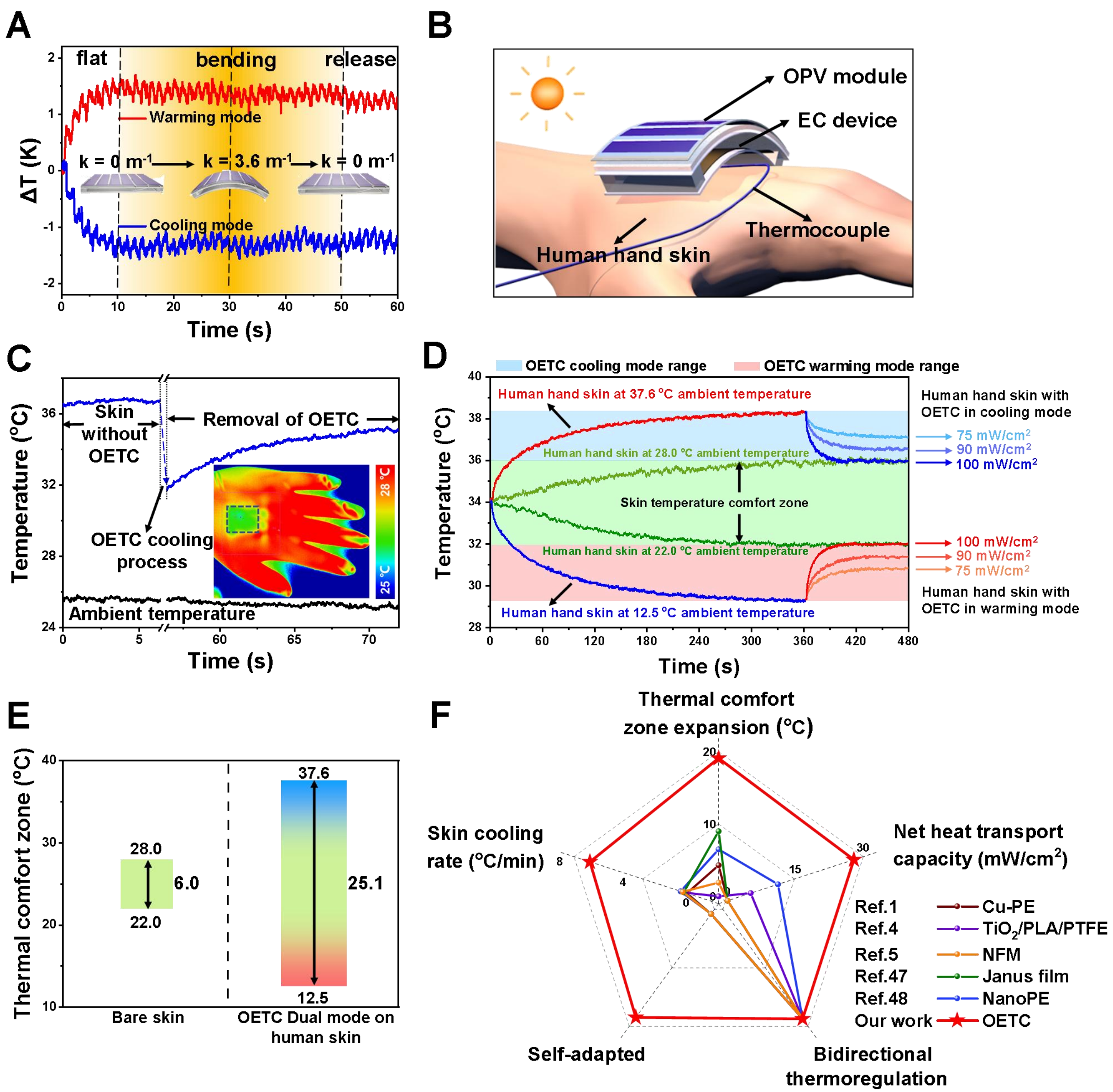
Working mechanism of OETC system in cooling/warming mode

Integrated OETC (OPV+EC)



Self-sustaining personal all-day thermoregulatory clothing using only sunlight

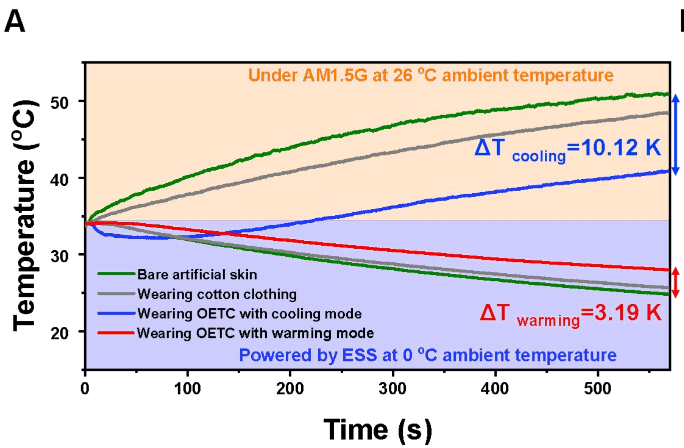
OPV+EC
集成器件



Self-sustaining personal all-day thermoregulatory clothing using only sunlight

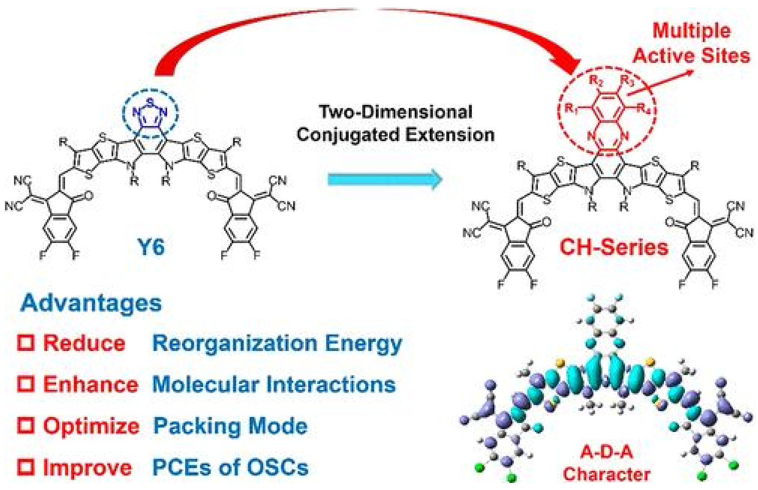
Thermoregulation performance of OETC in the outdoor and the prospect for use in space

OPV+EC
集成器件



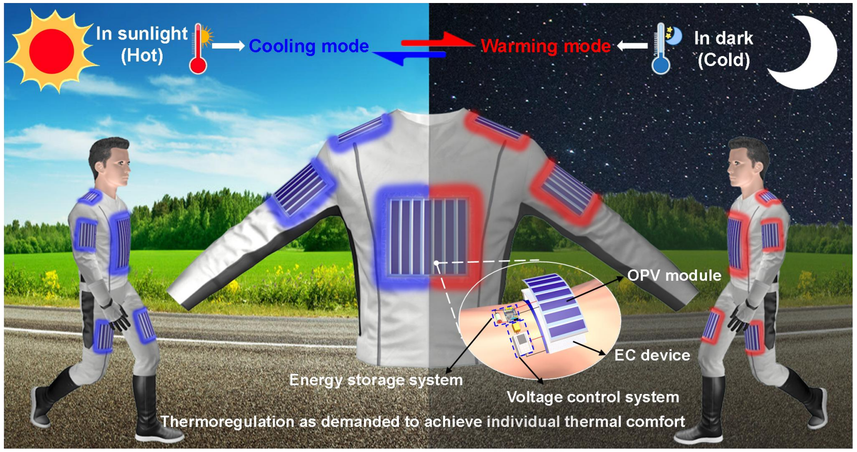
Summary

CH series of OPV molecules



***Acc of Mater Res*, 2023**, 4, 772
***Chem Soc Rev*, 2020**, 49 (9), 2828
***Acc Chem Res*, 2012**, 46, 2645

Flexible and wearable OPV devices



Cooling in sunlight, warming in dark!

Science, 2023, 328, 1291-1296

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Comments and Discussion welcomed