合肥微尺度物质科学
国家研究中心

HFNL, USTC

物理学院
《近代物理进展》专题报告

有机分子电子激发态的光物理过程和谱学表征

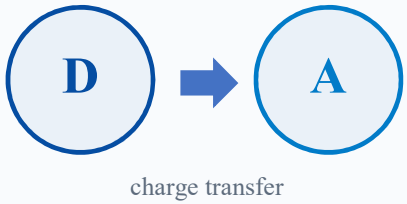
Electronic Excited-State Molecular Photophysics and Spectroscopic Characterization

从激发态动力学到手性自旋

From Excited-State Dynamics to Chiral Spin

报告人：张国庆 PhD, Professor of Chemistry

对象：物理学院一年级研究生新生 ·

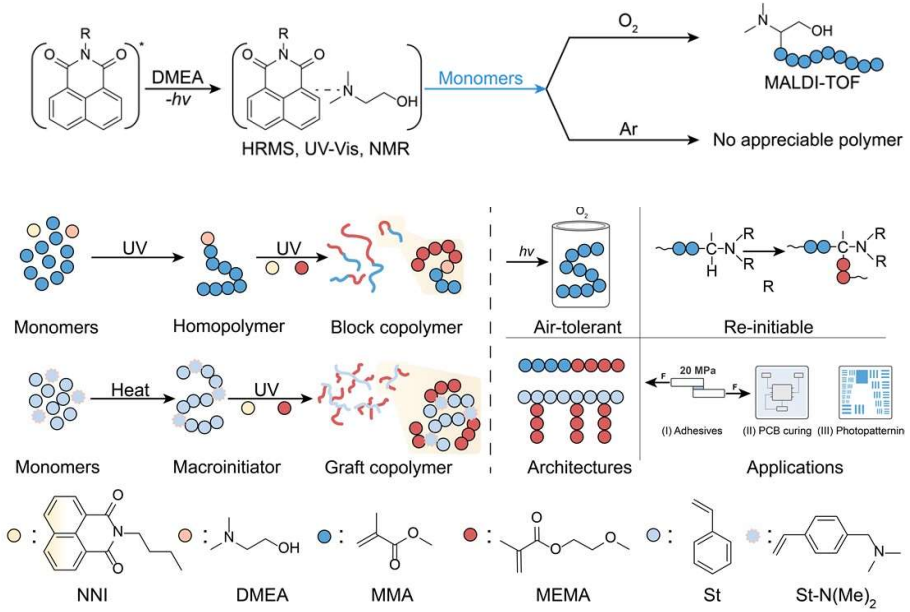


2026 年 11 月 12 日 · 7：00 PM@东区5301

课题组研究方向介绍：基础科学研究

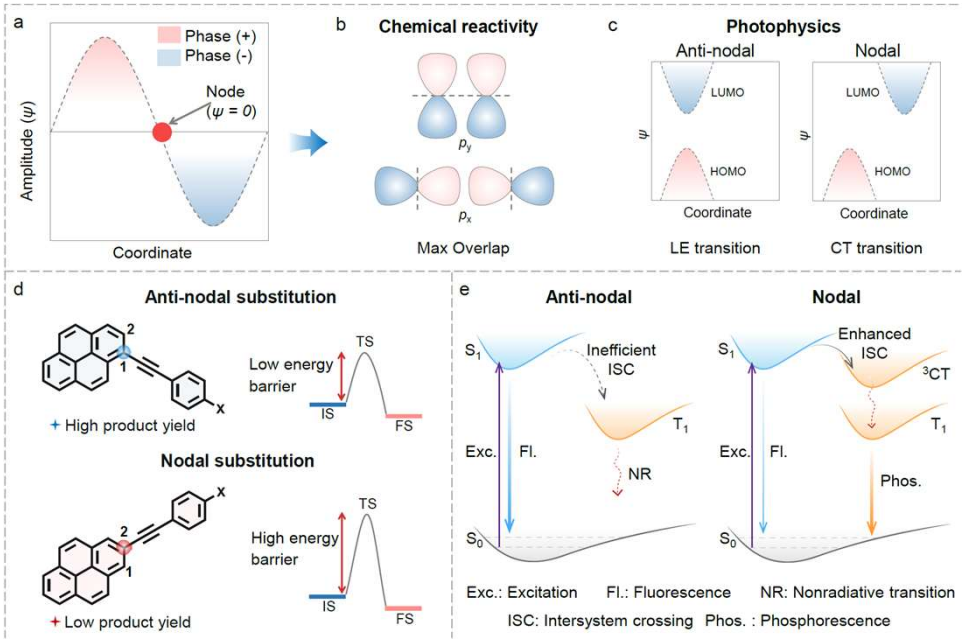
Research Directions

Polymer Chemistry (2011-)



2024年，课题组首先发现并且命名了了“光致基态电荷转移络合物”(*Chem*, **2024**, *10*, 2829; *J. Am. Chem. Soc.*, **2025**, *147*, 13512),并且实现了氧气激活的自由基聚合方法学，目前被成功用于新一代的光固化技术。

Molecular Photophysics (2011-)

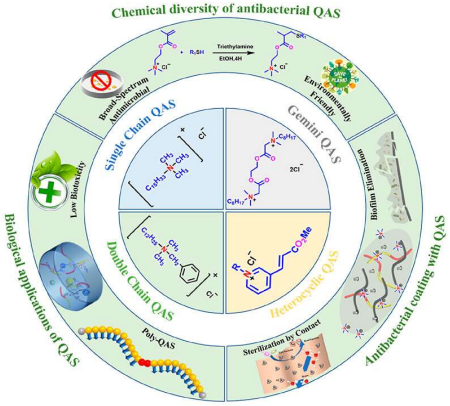


课题组在过去15年中，在有机分子的电子激发态和激发态自旋动力学理论、分子设计和谱学表征方向发表了一系列成果，包括*Nat. Commun.* 7篇，*Angew. Chem.* 11篇等论文。

课题组研究方向介绍：社会与经济效益

Research Directions

New Antiseptic Design (2015-)



Bioconjugate Chem. **2023**, 34, 2, 302–325



国家疾病预防控制局
新消毒产品卫生许可批件

共 2 页 第 1 页

产品名称	蓝杉®埃芙莫拉消毒液	
产品类别	消毒剂	
剂型或型号	液体	
生产企业/在华责任单位	名称	安徽启威生物科技有限公司
	地址	安徽省合肥市高新区创新大道106号明珠产业园5号楼二层A、B区
实际生产企业	安徽启威生物科技有限公司	
实际生产企业地址	安徽省合肥市高新区创新大道106号明珠产业园5号楼二层A、B区	
审批结论	经审核，该产品符合《新消毒产品和新涉水产品卫生行政许可管理规定》《利用新材料、新工艺技术和新杀菌原理生产消毒剂和消毒器械的判定依据》的有关规定，现予以批准。	
批准文号	国疾控消新字（2024）第0001号	
批准日期	2024年8月14日	
批件有效期	截至 2028年8月13日	
附件	产品说明、使用范围、使用方法和注意事项	

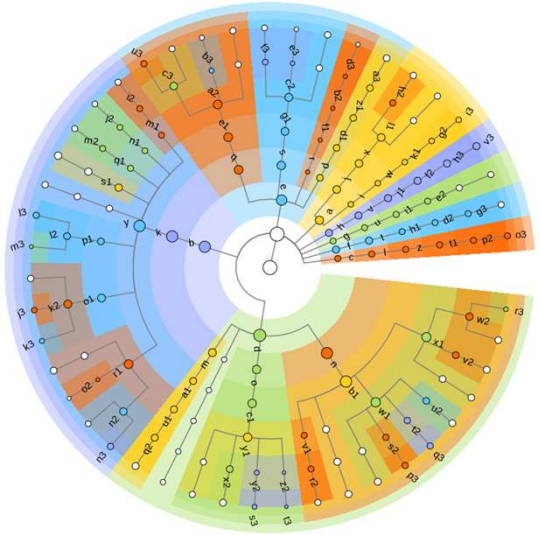
注：请于批件有效期届满30个工作日之前向省级疾病预防控制部门备案。

批准机关
2024年8月14日

1

埃芙莫拉®消毒液正式获得国家疾病预防控制局新消毒产品卫生许可批件文号“国疾控消新字（2024）第0001号”，首个“三新”消毒产品。

Clinical Trials of New Drug (2022-)



中科大张国庆课题组、安徽启威生物科技有限公司和东阳光集团（600673）合作开发的原研药先导化合物即将进入临床申报阶段，入选2027科技春晚成果介绍。

课题组研究方向介绍：国家战略方向布局

Research Directions

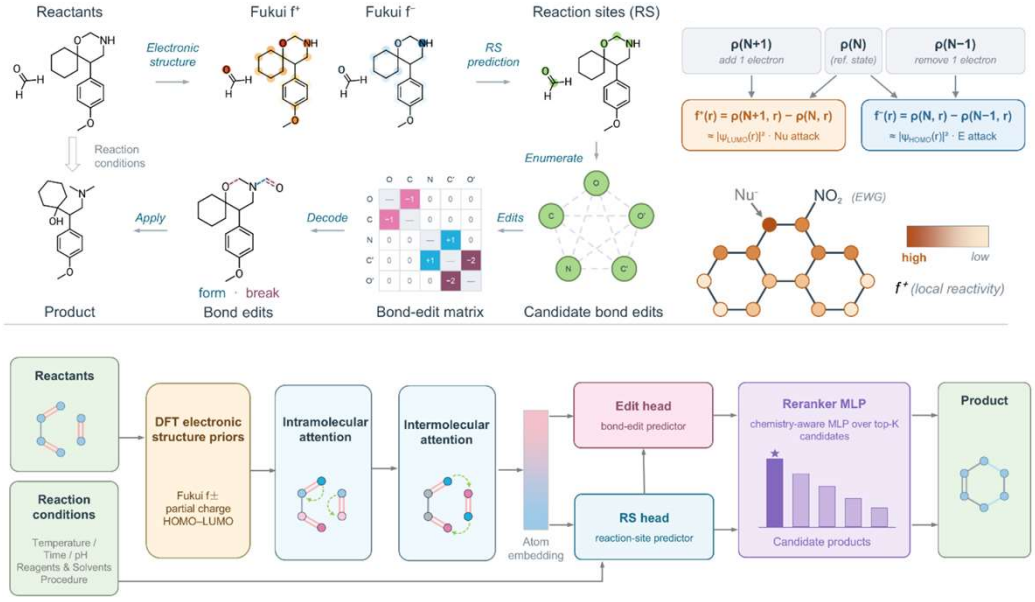
Automated Chemistry Lab (2024-)



自动化高通量实验谱学平台

东区物质楼BC105实验室

Retro/Forward Chemistry Prediction (2021-)



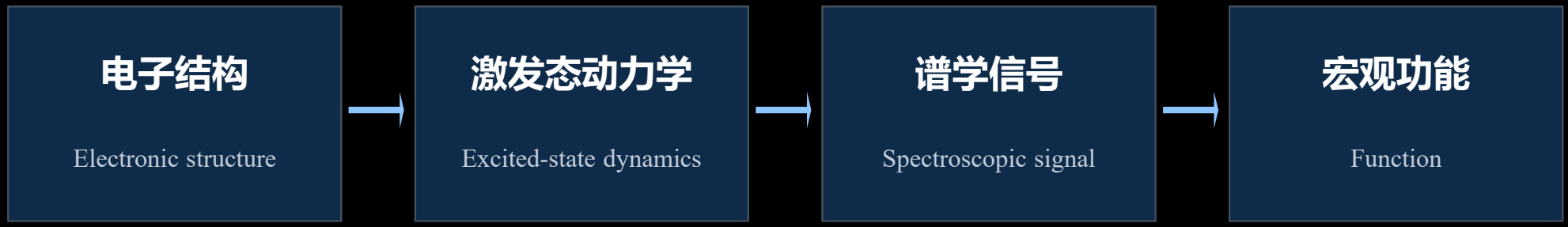
基于量子化学规则的预训练

真实场景下达到>95%的预测准确率

电荷转移不是终点，而是激发态动力学的起点

Charge Transfer as the Starting Point of Excited-State Dynamics

光致电荷转移伴随能量传递与自旋演化，直接决定分子的反应活性与光物理性能。



核心任务：建立“分子 / 电子结构—时间分辨谱学—宏观光学性质”的可信关联。

来源：张国庆，国家自然科学基金申请书《有机激发态电荷转移动力学及手性自旋》（2026 版），报告正文。

01

近代物理进展 · 专题报告 / MODERN PHYSICS PROGRESS

新物种：突破电荷转移的二元分类

A NEW SPECIES: BEYOND THE BINARY CLASSIFICATION

能否让光照成为复合物形成的必要条件，并把光子能留到黑暗中使用？

Benesi 和 Hildebrand 研究了碘和溶剂间的电荷转移复合物（CTC）

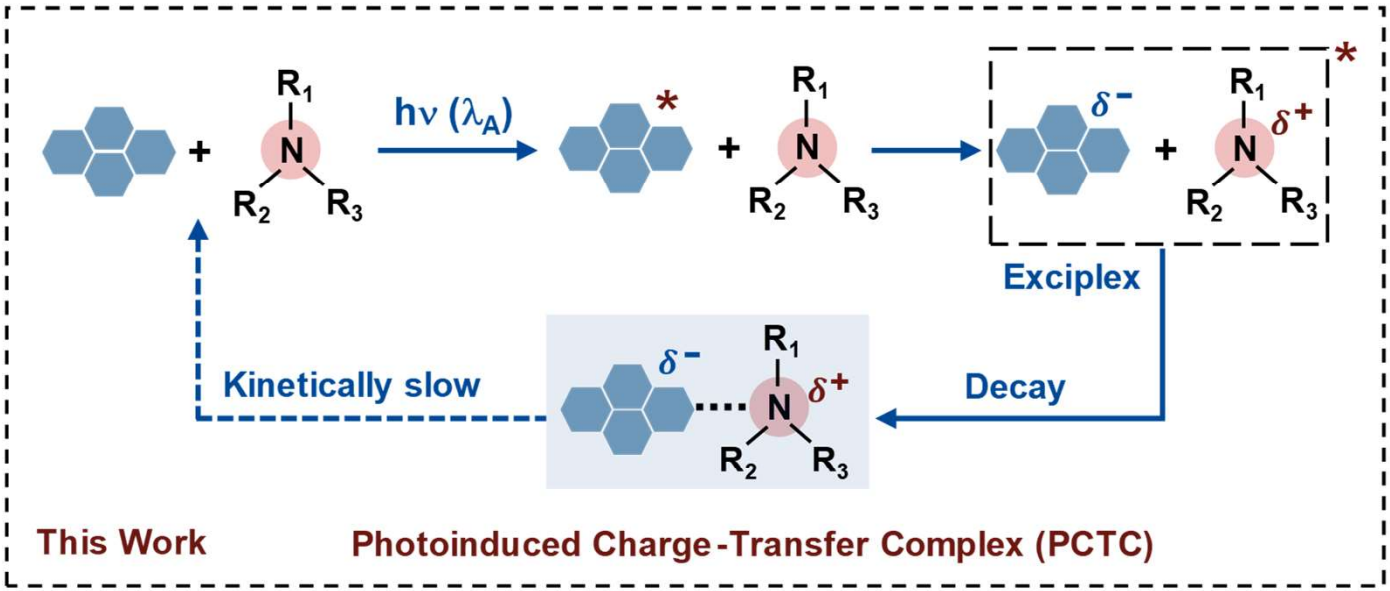
Förster 和 Kaspar 研究了芘分子形成的excimer

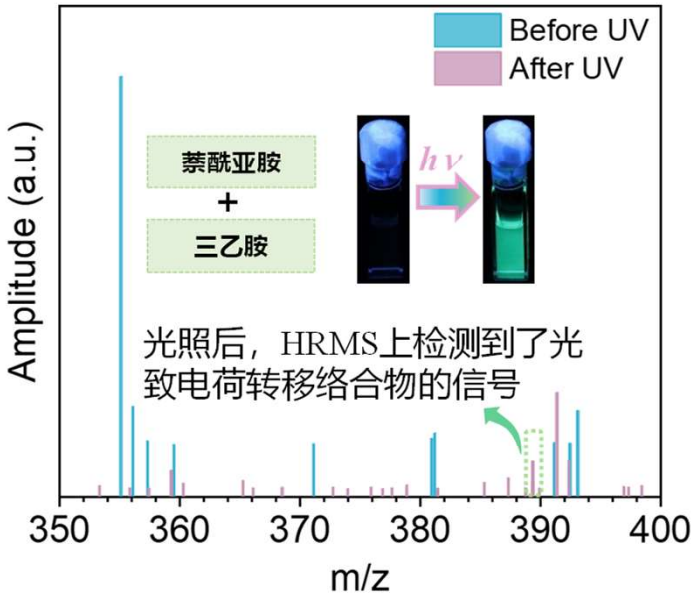
Leonhardt 和 Weller研究了芘和二甲基苯胺的exciplex

1949年：基态电荷转移络合物

1954年：同分子激基缔合物

1963年：异种分子激基缔合物





2024年, 张国庆课题组发现第一个异种分子的光致基态电荷转移络合物———萘酰亚胺和三乙胺的 PCTC

Why Do Two Neutral Molecules Associate?

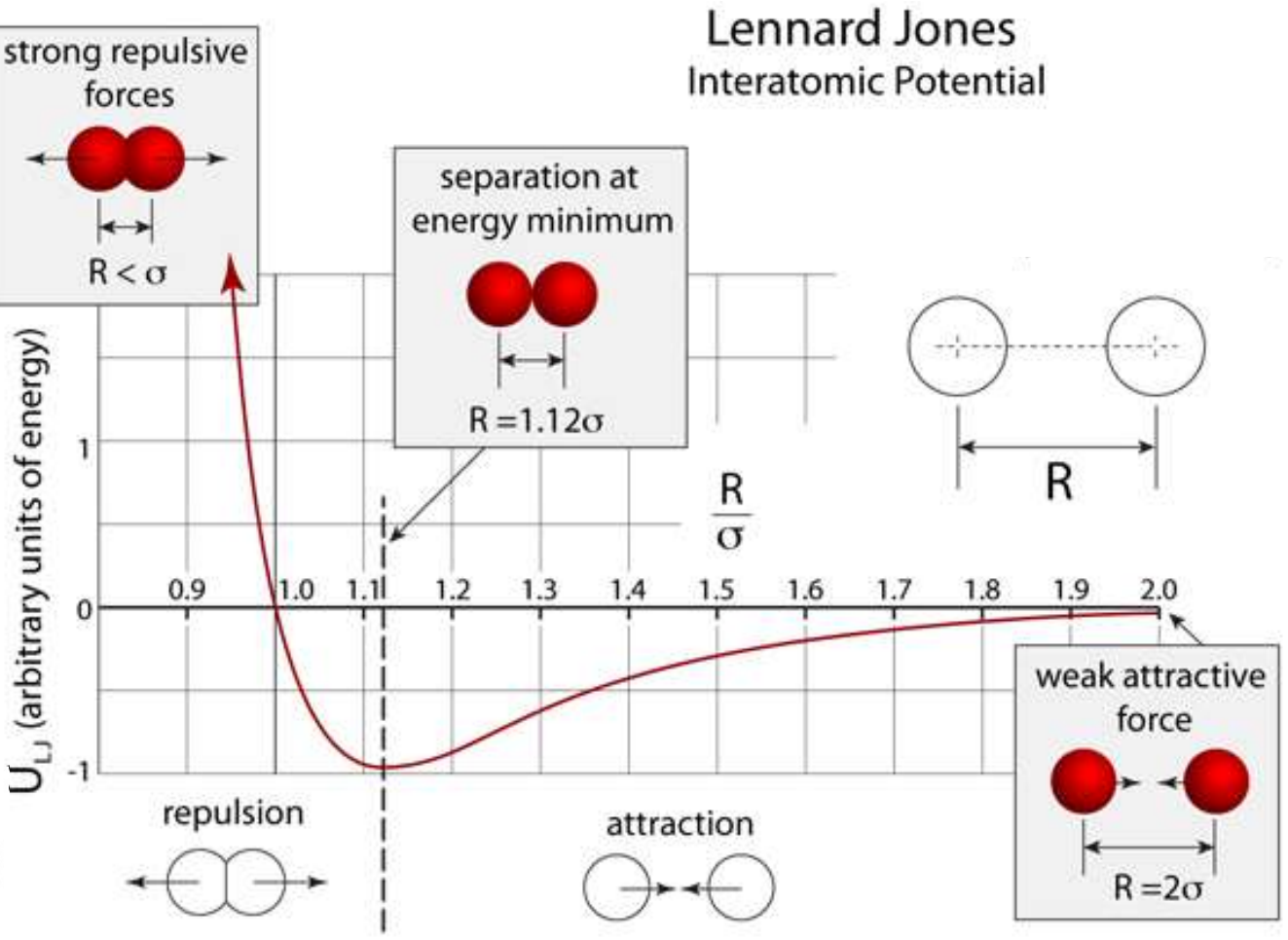
Lennard-Jones potential for describing the interaction between a pair of neutral atoms or molecules

$$E(r) = \frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}$$

Pauli Exclusion

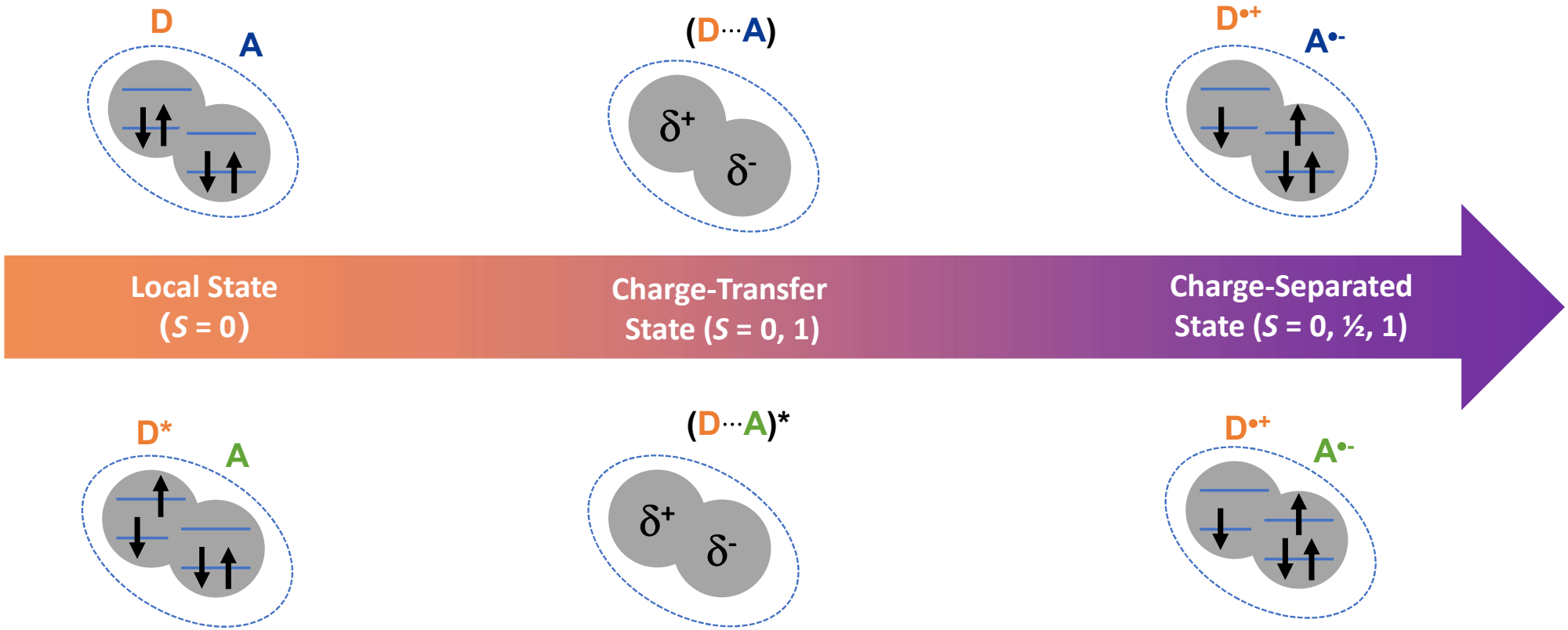
London Dispersion

$$E_{\text{Buckingham}}(r) = A \exp\left(-\frac{r}{\rho}\right)$$

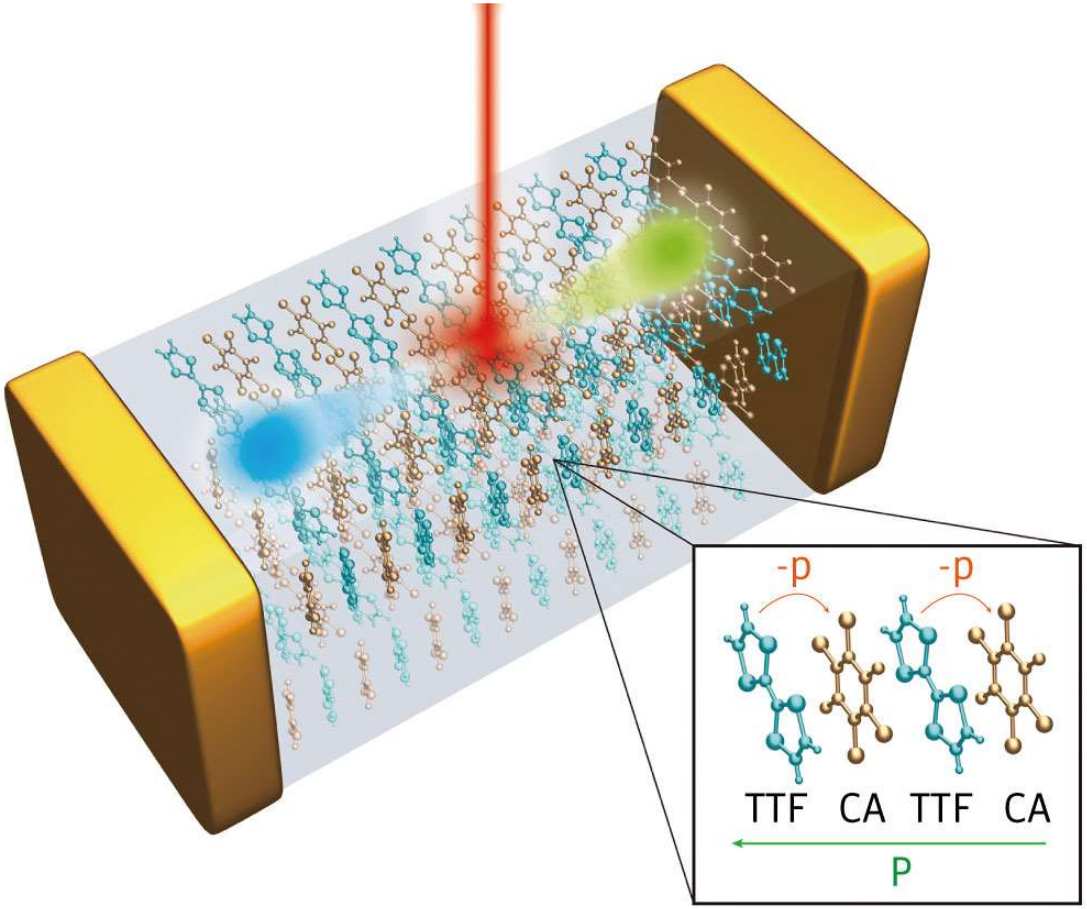


Charge Transfer: Reduced “Pauli Repulsion”

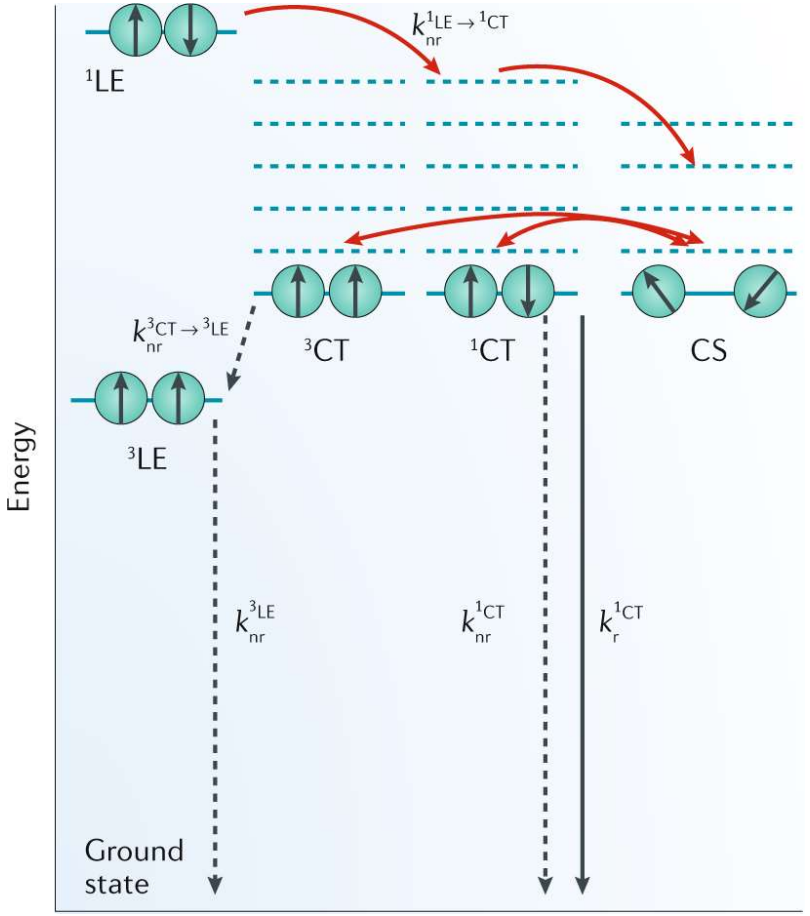
In molecular systems, charge transfer (CT) states are broadly defined as bound combinations of an electron and **a hole** located on separate molecules or moieties before reaching complete charge separation. It is generally an intermediate state.



Why Do We Care About Excited-State Charge Transfer?

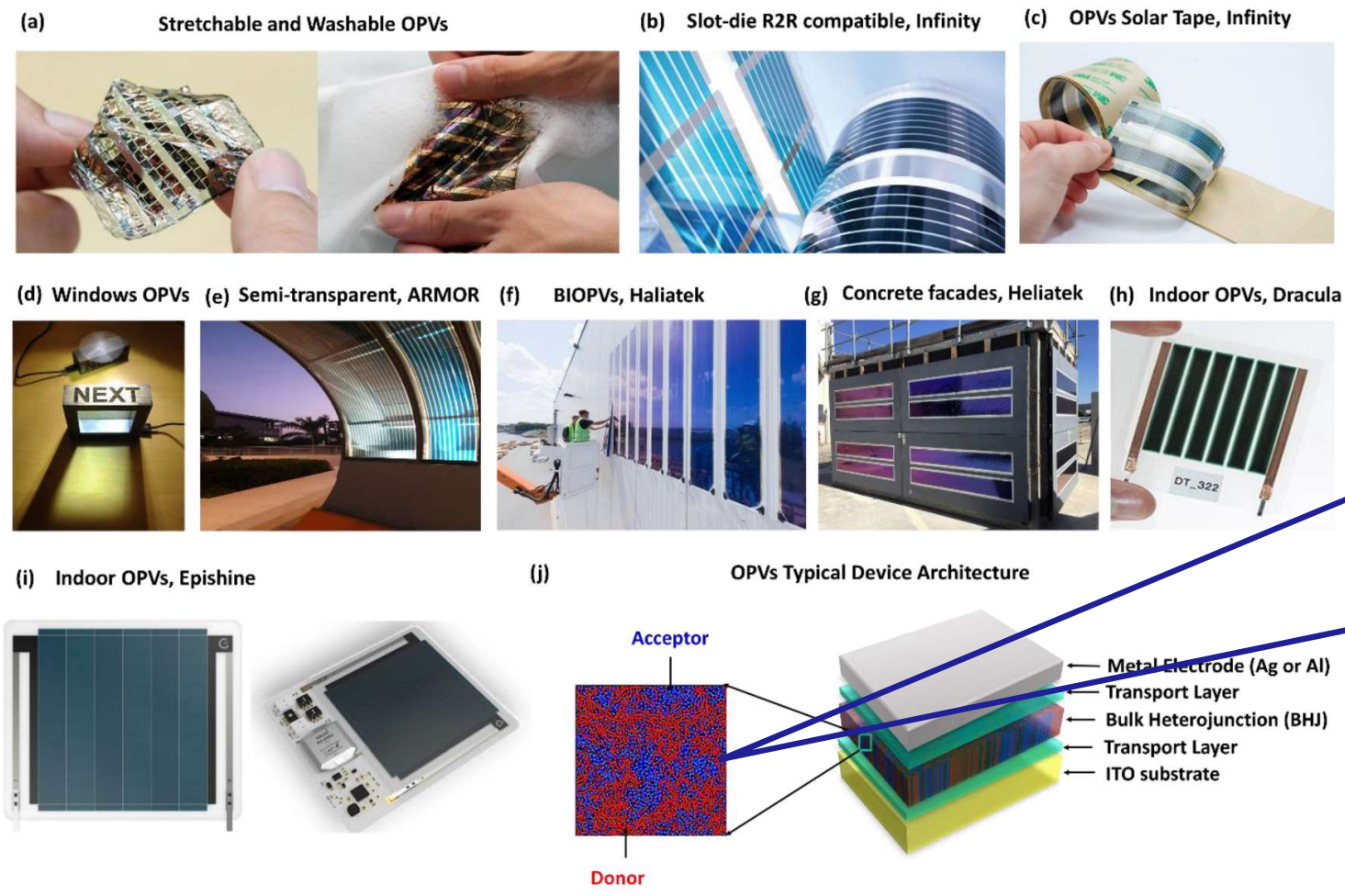


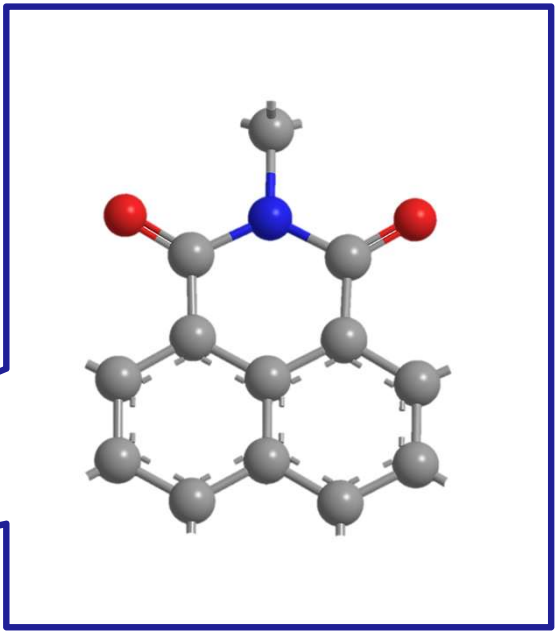
Nakamura et al., *Nat. Commun*. **8**, 281 (2017).



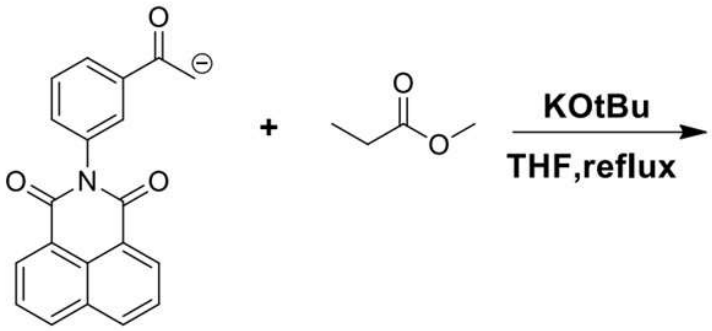
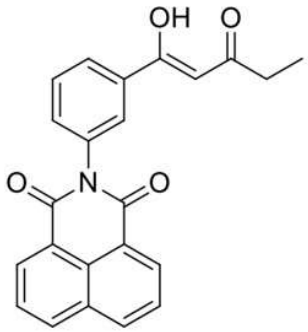
Coropceanu, V. et al. *Nat. Rev. Mater.* **4**, 689 (2019)

Naphthalimide As Model Acceptor





The Discovery

Reaction[a]	Expected product	^{1}HNMR	ESI-MS
		Not found	Not found

Claisen Condensation
Summer of 2017

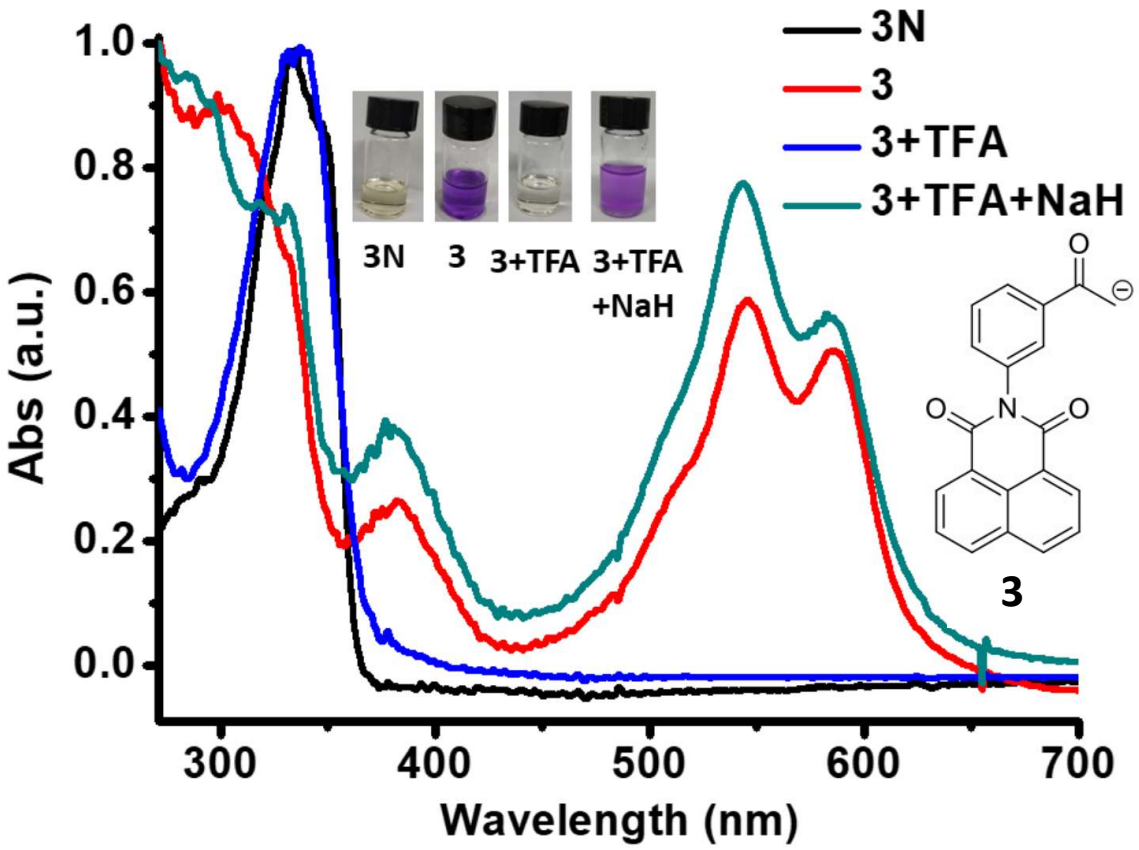


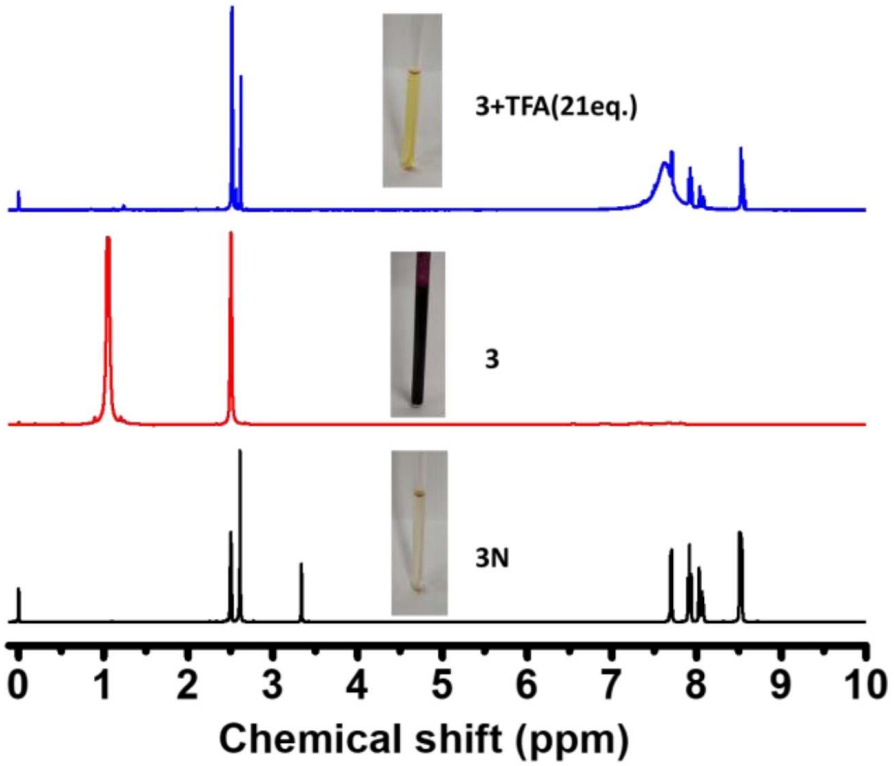




Relatively stable under air after 1 day

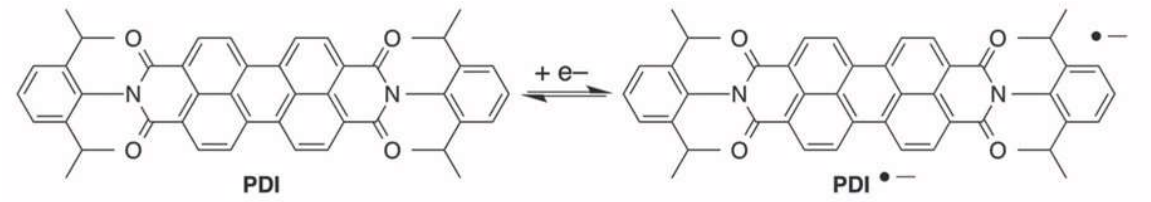
Reversible Deprotonation-Protonation Cycle

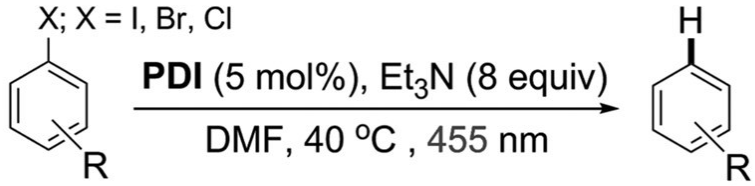


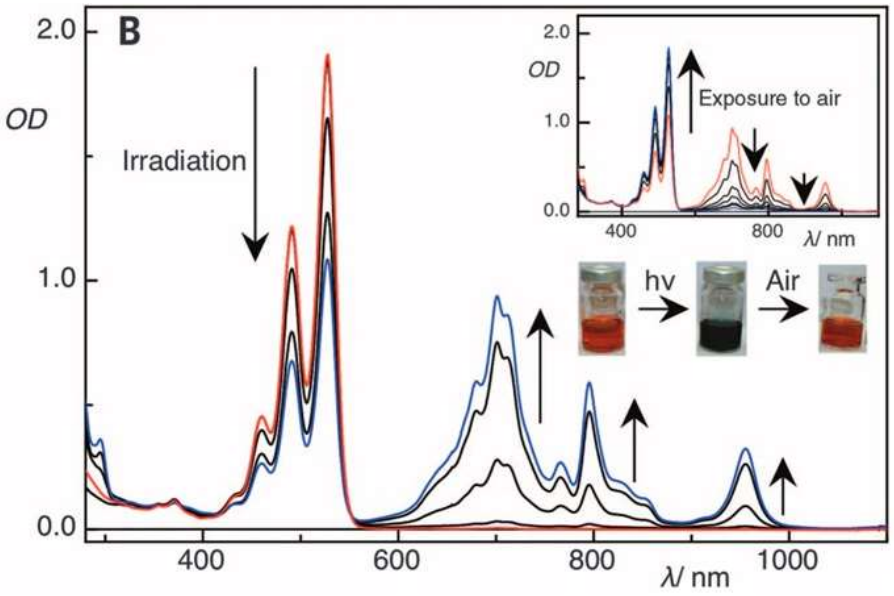


Chem. Eur. J., **2019**, *25*, 12497, Hot Paper

Radical Anion Mechanism







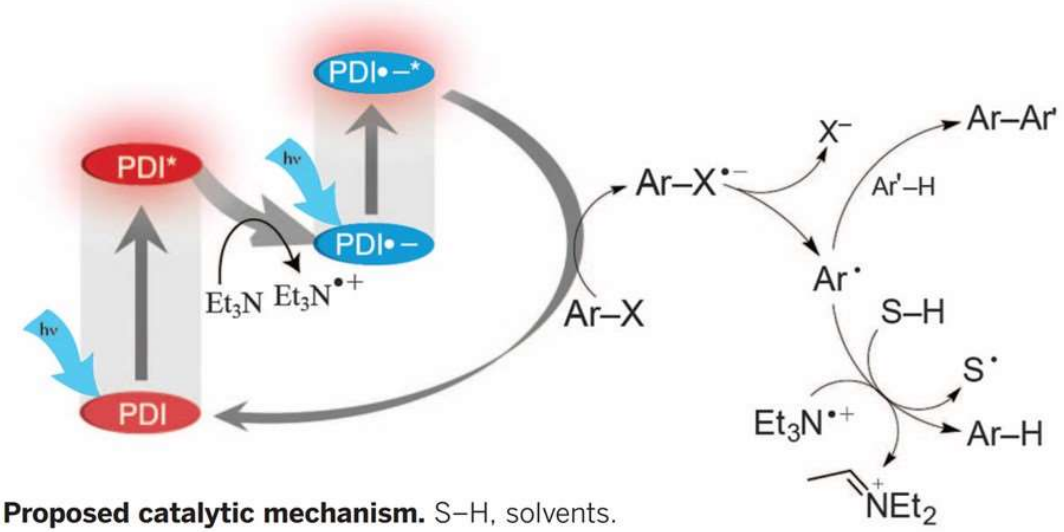
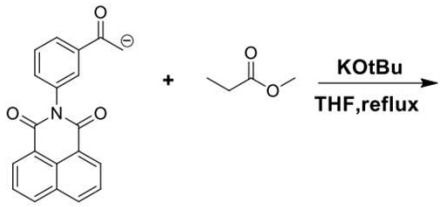
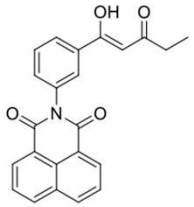
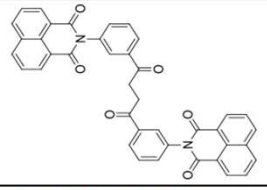
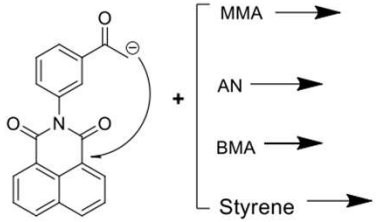
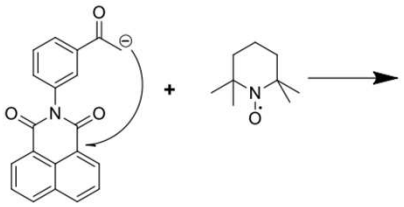
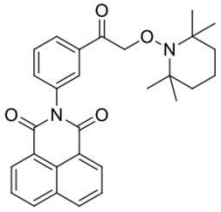
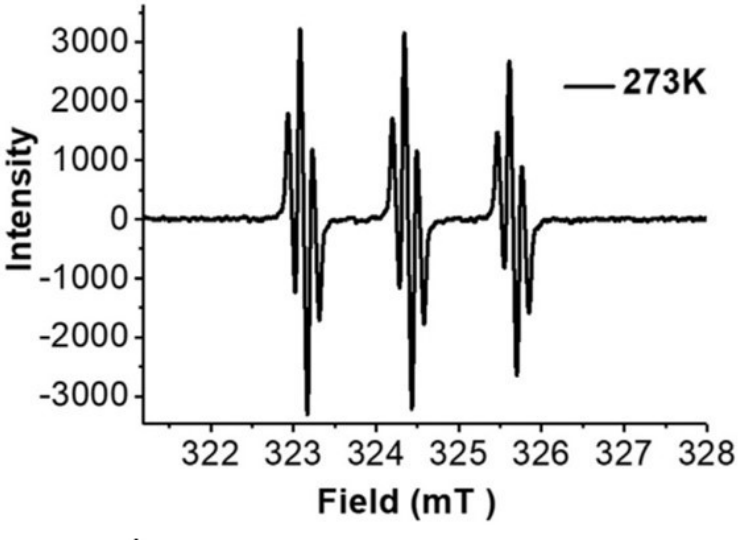


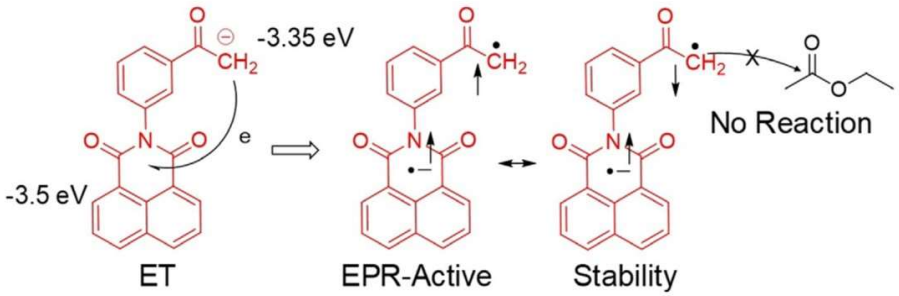
Fig. 4. Proposed catalytic mechanism. S–H, solvents.

Ghosh *et al.* Reduction of aryl halides by consecutive visible light-induced electron transfer processes. *Science* **2014**, *346*,725-728 (2014).

Persistent Diradical-Like Species?

Reaction[a]	Expected product	^{1}HNMR	ESI-MS
		Not found	Not found
		Not found	Not found
	PMA/PAN/PBMA/PS	Not found	Not found
		Not found	Not found

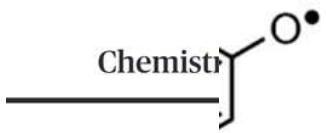




Chem. Eur. J., **2019**, *25*, 12497, Hot Paper

Chem. Eur. J., **2020**, *26*, 12743

Explanation Met with Peer Criticism



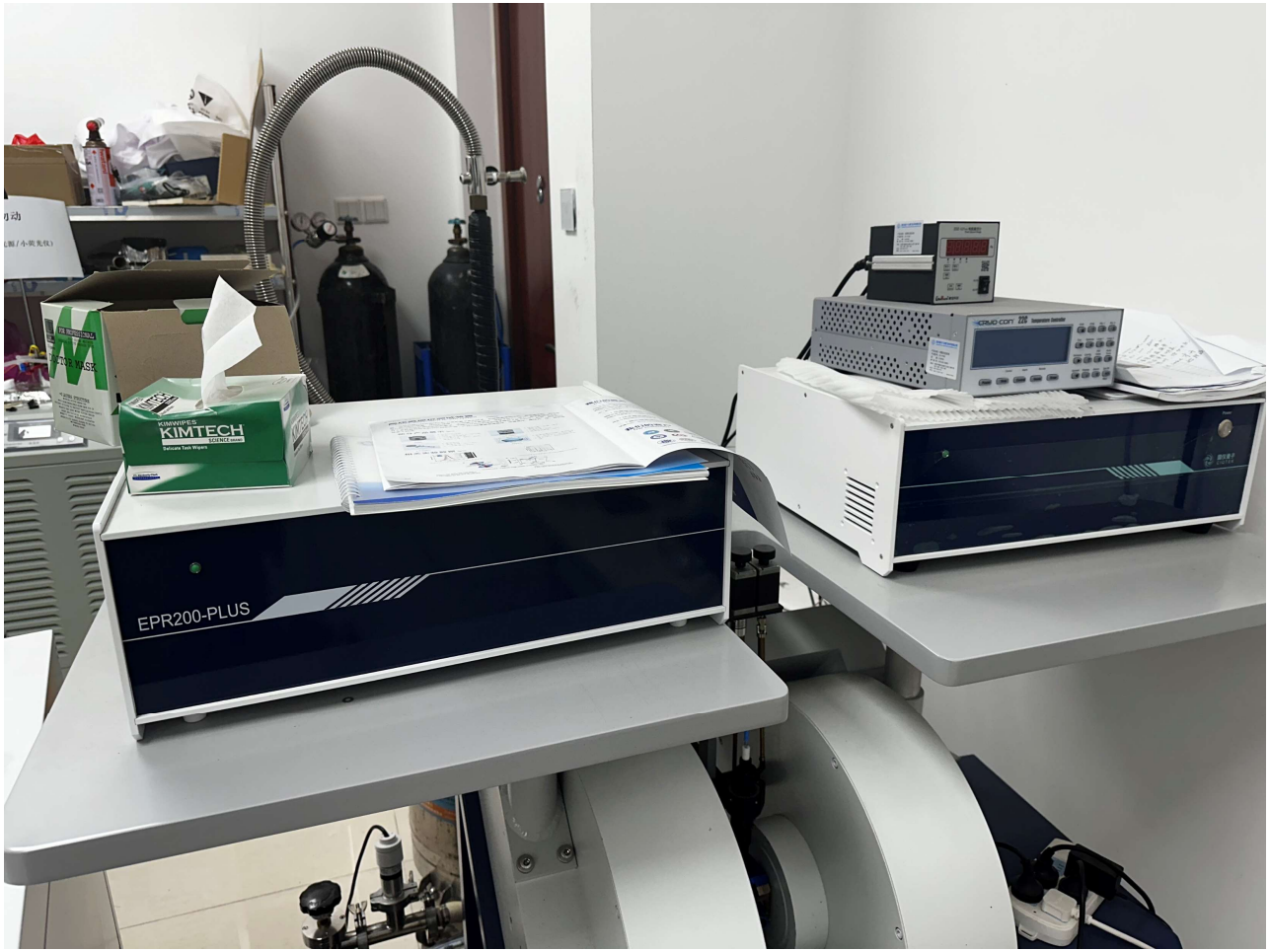
Second, the authors of ref. [1] do not seem to consider (or to be aware of) the fact that EPR spectrometry is much more sensitive than, for example, NMR. Thus, as experienced for decades, even minor (in the μM range) amounts of radical species may give rise to apparently strong EPR signals. It should also be noted that no attempts to determine radical concentrations were reported. Hence, the persistent nitroxide radical of Figure 2 b,c (ref. [1]) is likely to constitute a kinetically "late" species, formed via a complex reaction sequence, either from **3**, the solvent DMF, some contamination (e.g., unsubstituted naphthalimide), or some combination of those. In fact, KO*t*Bu-induced formation of (nitroxide-type) radicals,[12] including radicals from KO*t*Bu-DMF interactions,[13,14] has previously been reported, but convincing as-

Korth, *Chem. Eur. J.*, **2020**, *26*, 12747

Questionable EPR assignments and signals too weak for a concentration of 10^{-3} M!!!

"Kinetically late species" indicated by Korth NOT found for control samples without NNI.

Our Costly ($250 K) Response



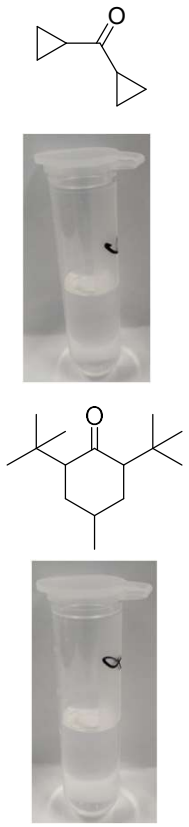
We believe we have a few possible answers now. However, the results are not ready for publication yet.

Characters of CT Complex

Enolate Donor



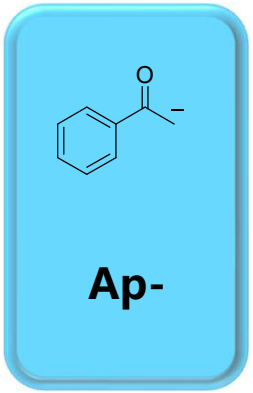
Sterics



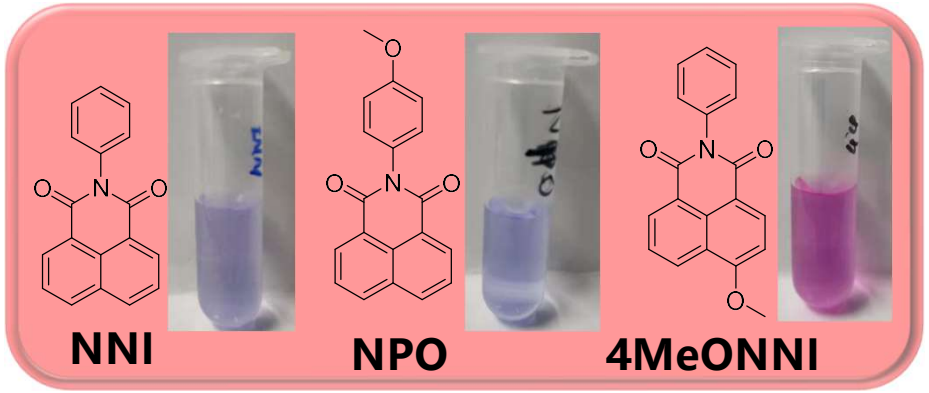
Counterion

Li+ Na+ K+





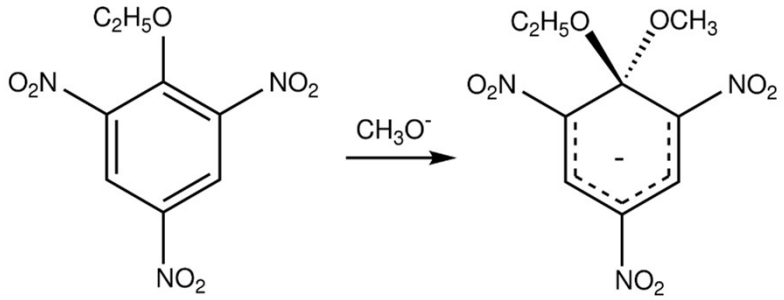
NNI Acceptor

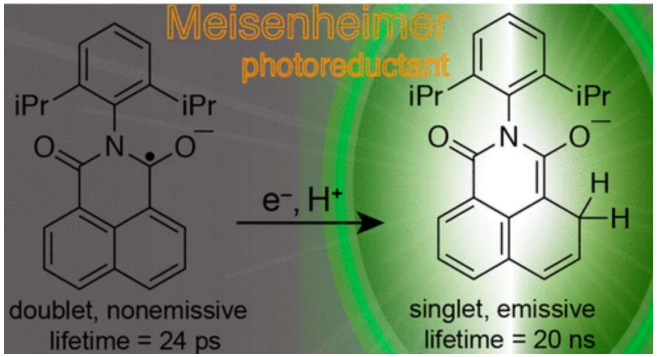


Unpublished results

Covalent Meisenheimer Complex

In 1886 Janovski observed an intense **violet color** when he mixed nitrobenzene derivative with an alcoholic solution of alkali. In 1902 Jakob Meisenheimer observed that by acidifying their reaction product, the starting material was recovered.



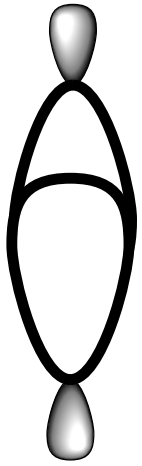


In 2021, the Nocera group reported an imide-based fluorescent Meisenheimer complex from NMR : *J. Am. Chem. Soc.* **2021**, *143*, 14352–14359

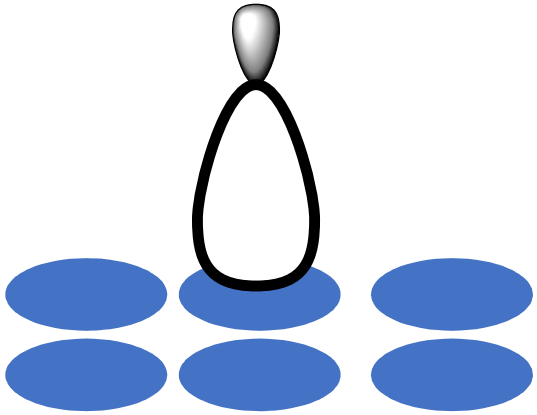
The loss of NMR spectra signals made the detective work very difficult.

The Overlap Integral Hypothesis

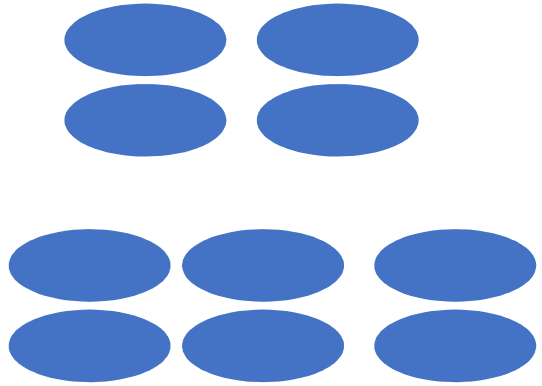
For a pair of donor-acceptor molecules, if the HOMO of the donor is higher than the LUMO of the acceptor:



σ donor and σ acceptor: chemical bonding

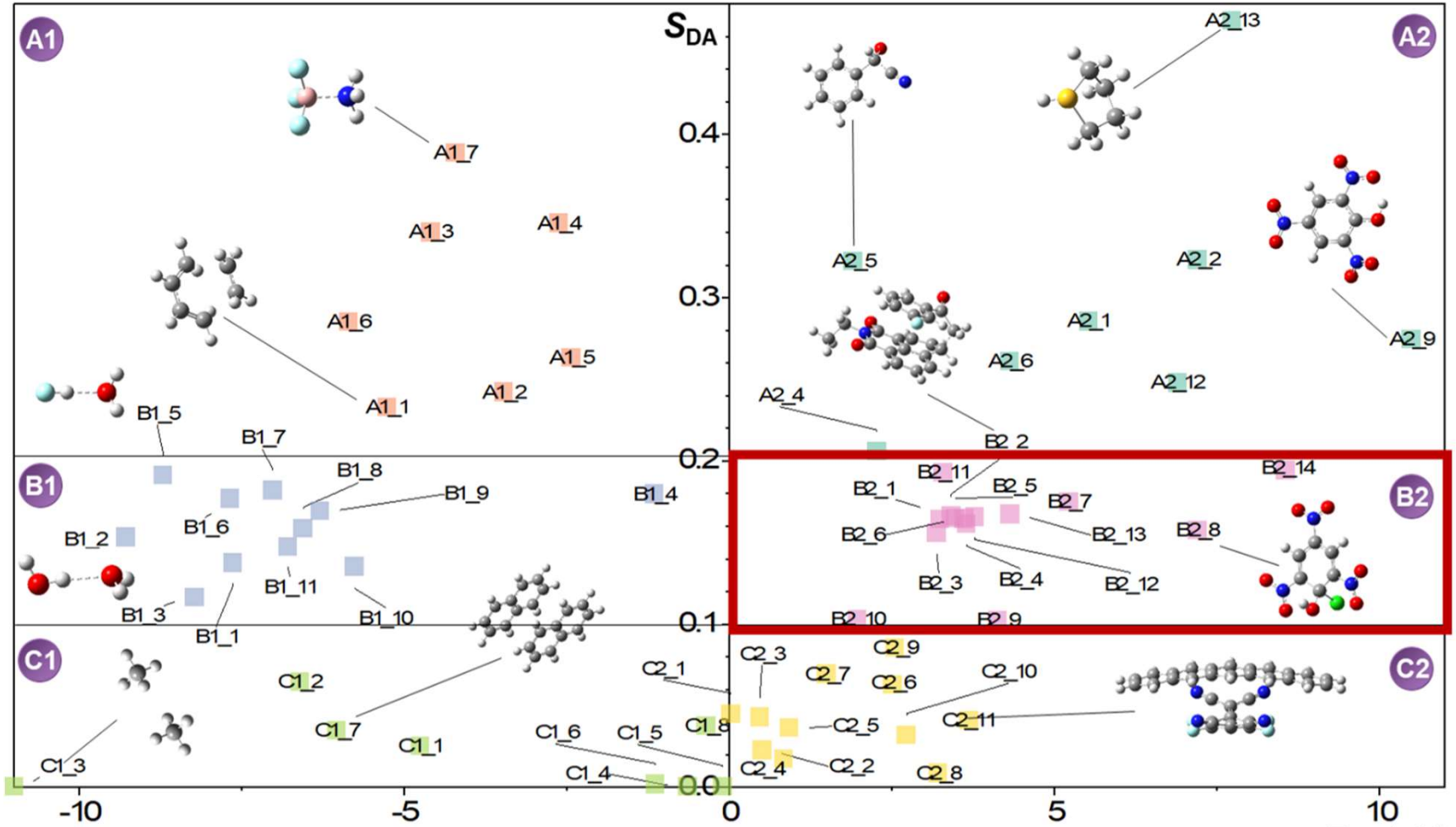


σ donor and π acceptor: Meisenheimer and Noncovalent



π donor and π acceptor: radical pair

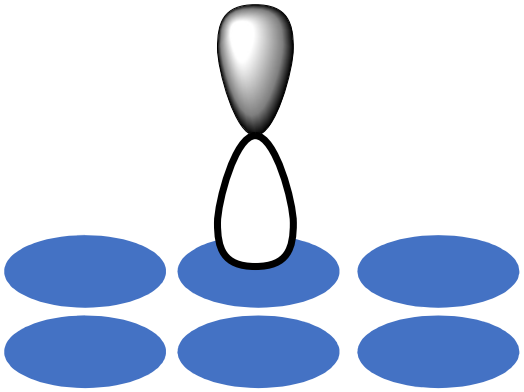
The Overlap Integral Hypothesis



https://pubs.rsc.org/en/content/articlelanding/2024/ra/d3ra07729b *ASAP*

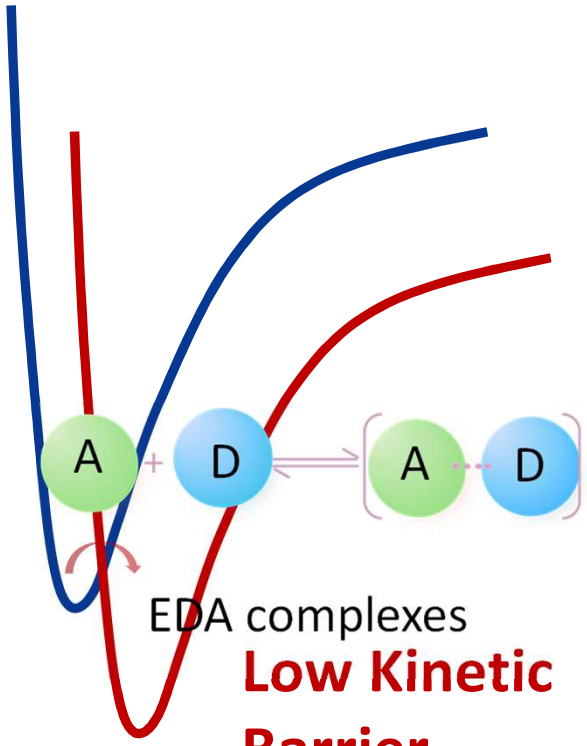
The Overlap Integral Hypothesis

σ-like donor



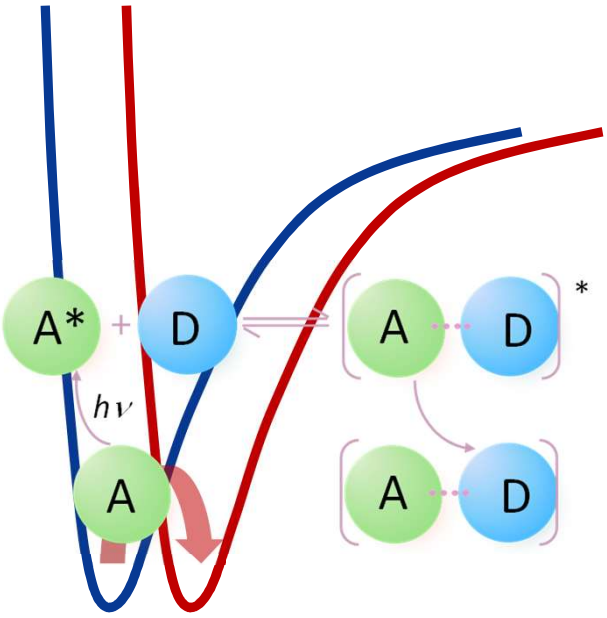
π*-like acceptor

Spontaneous Complex Formation



Low Kinetic Barrier

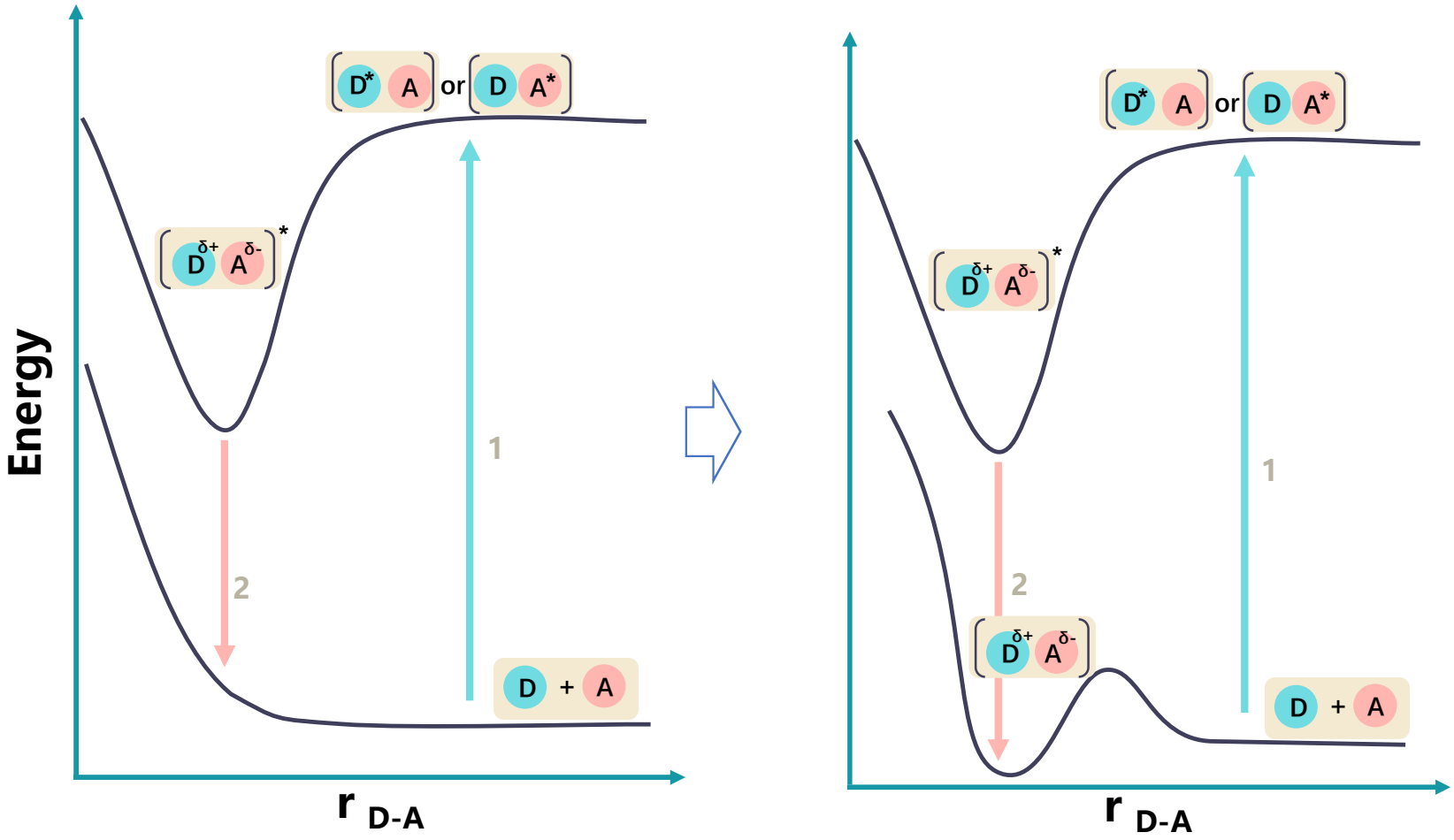
Activated Complex Formation?



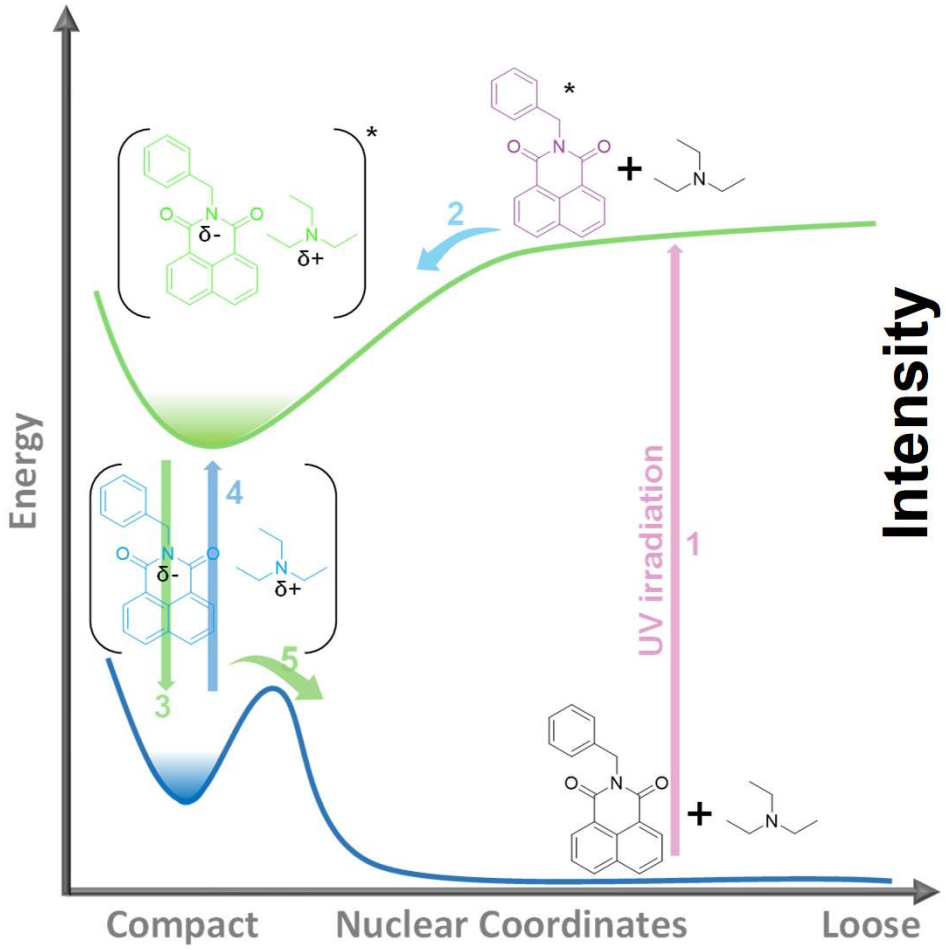
High Kinetic Barrier

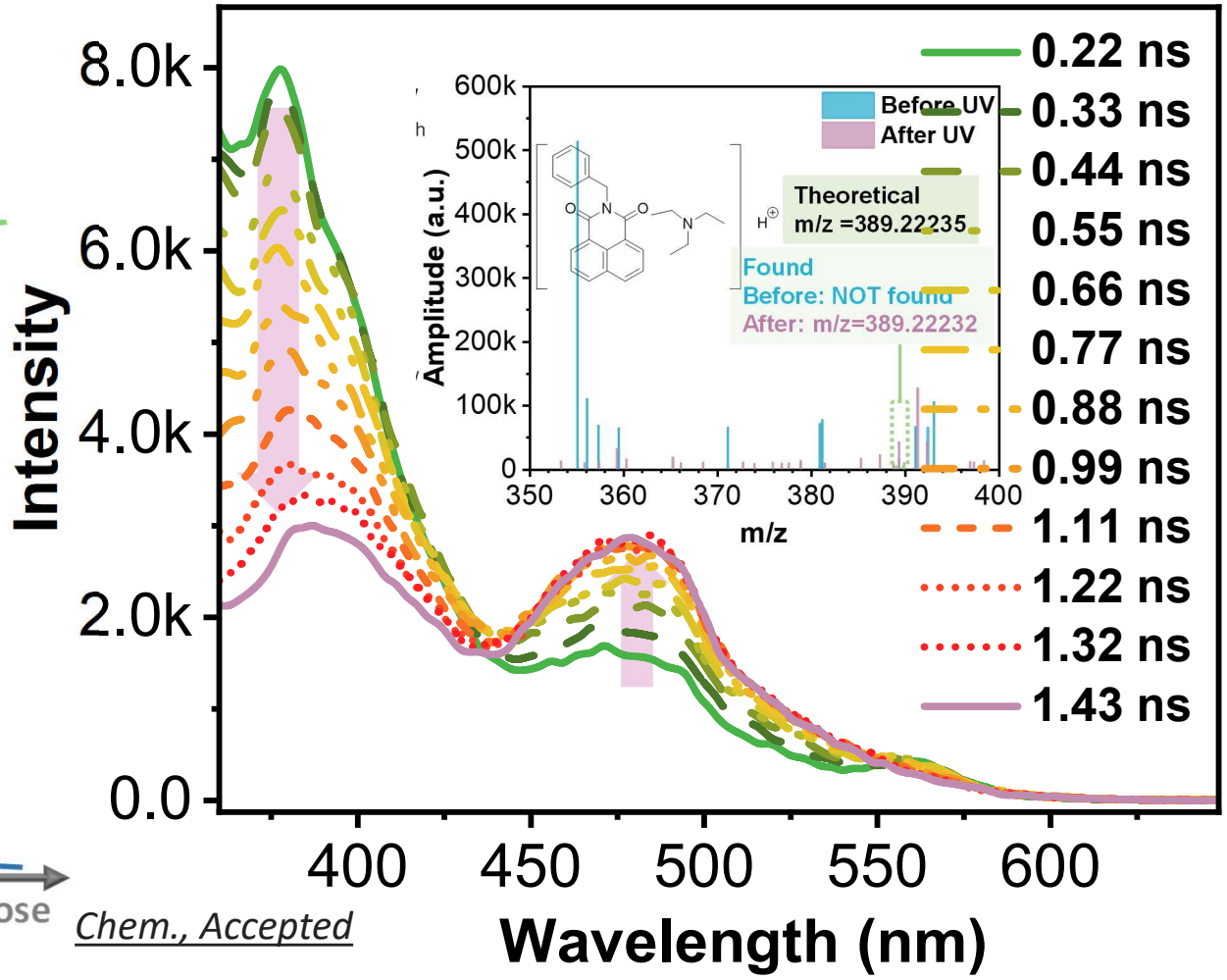
Chem., Accepted

Photo-Induced Charge-Transfer Complexes



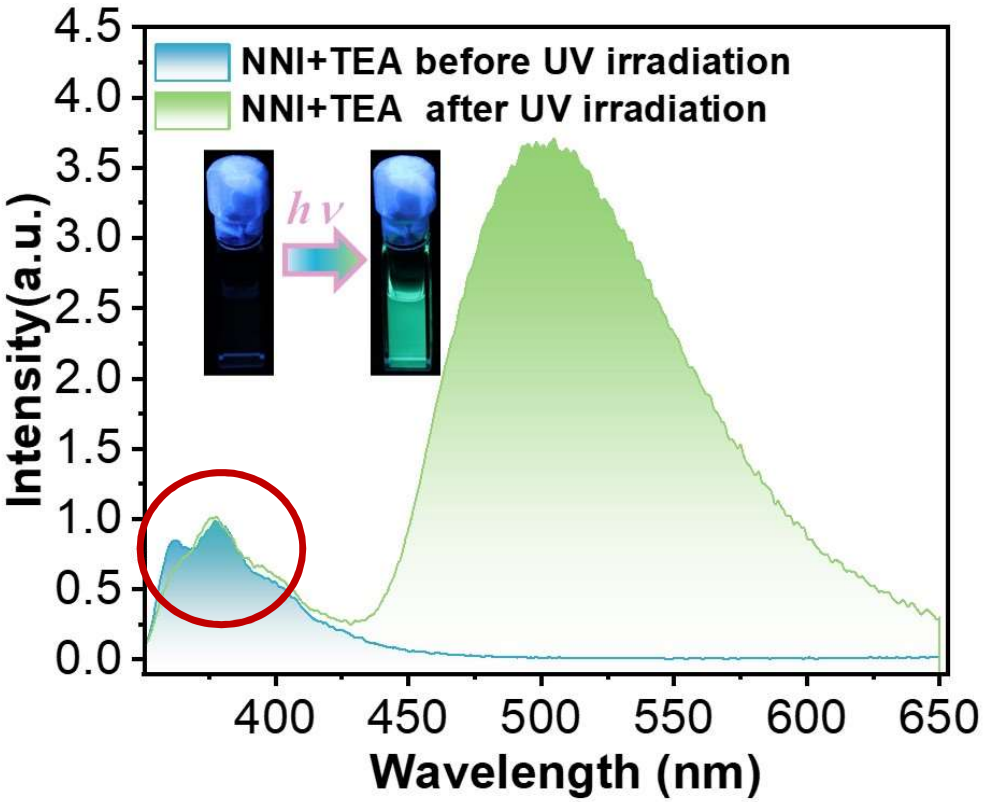
Spectroscopic Evidence

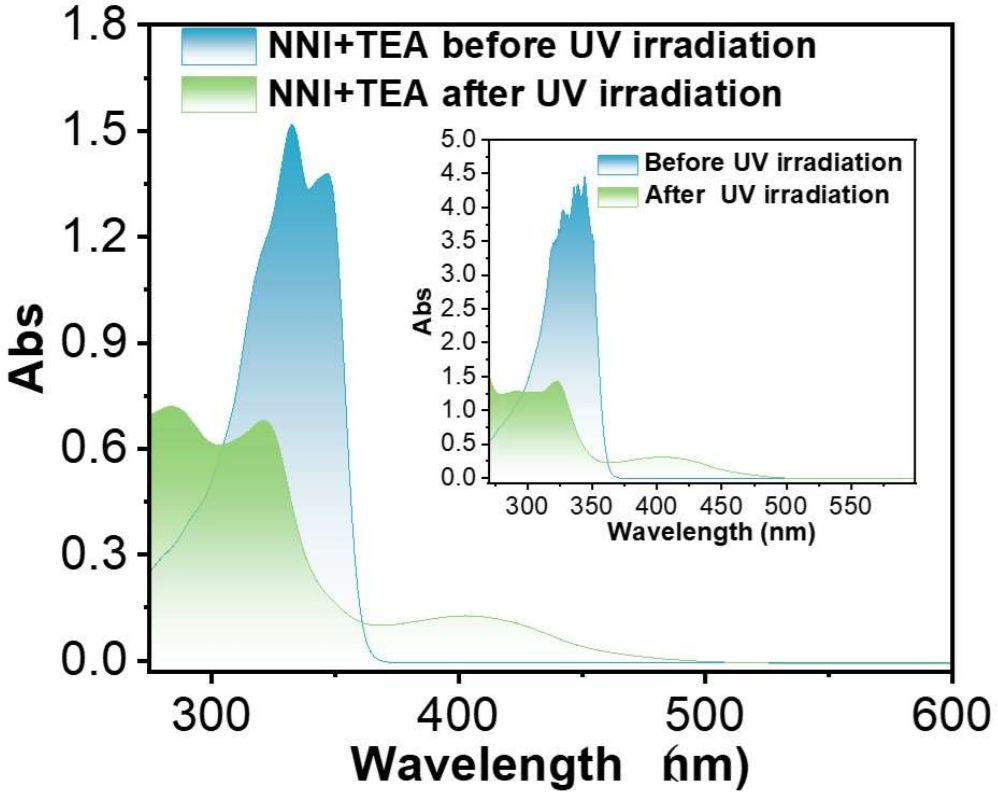




Chem., Accepted

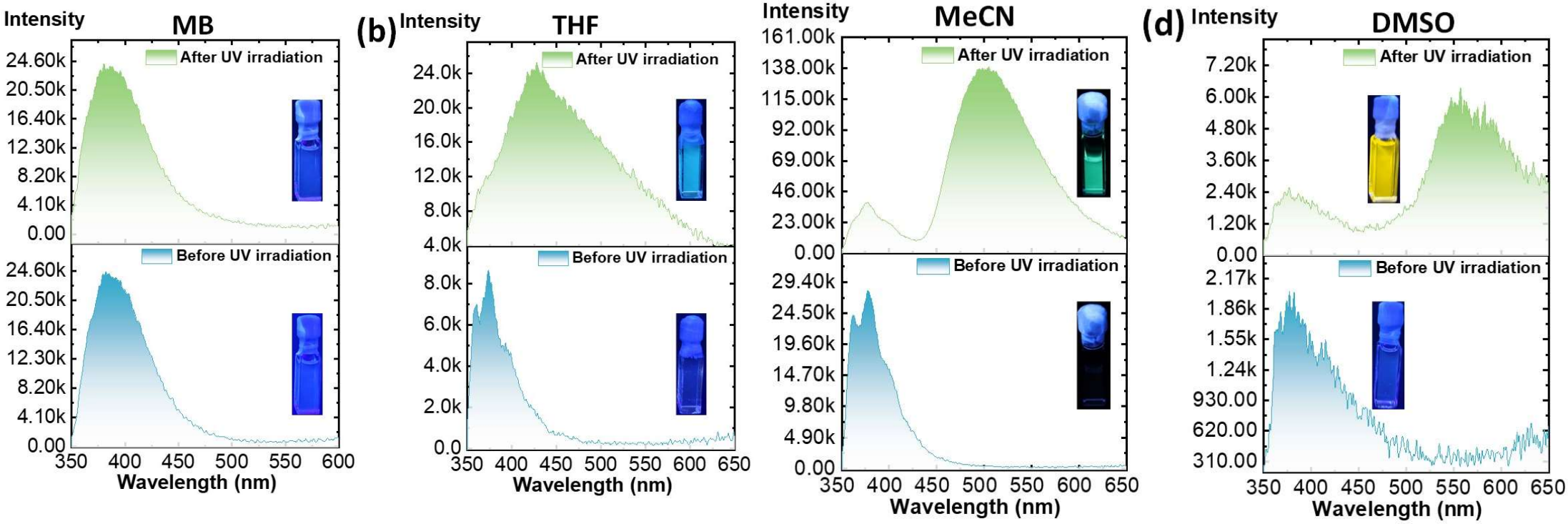
Physical Properties of PICTC





There is a change in the 0-0 to 0-1 ratio: Not residual NNI emission.
Decreased I^{0-0}/I^{0-1} indicates dimer formation.

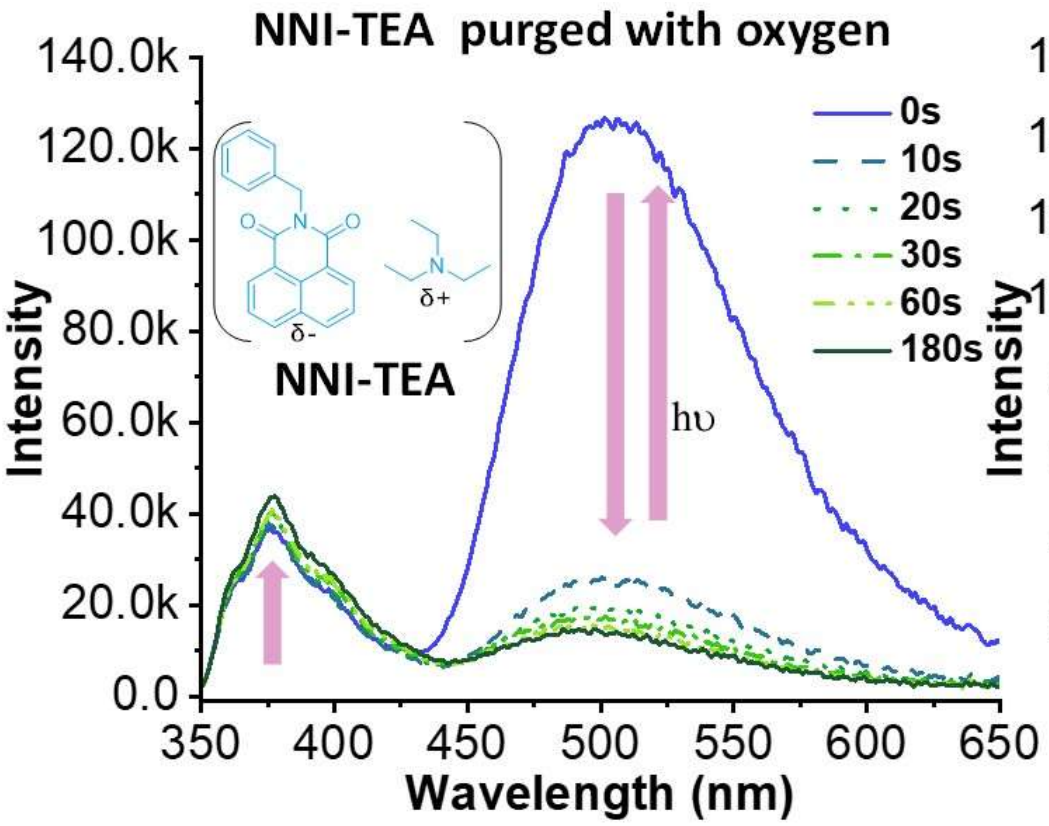
Physical Properties of PICTC

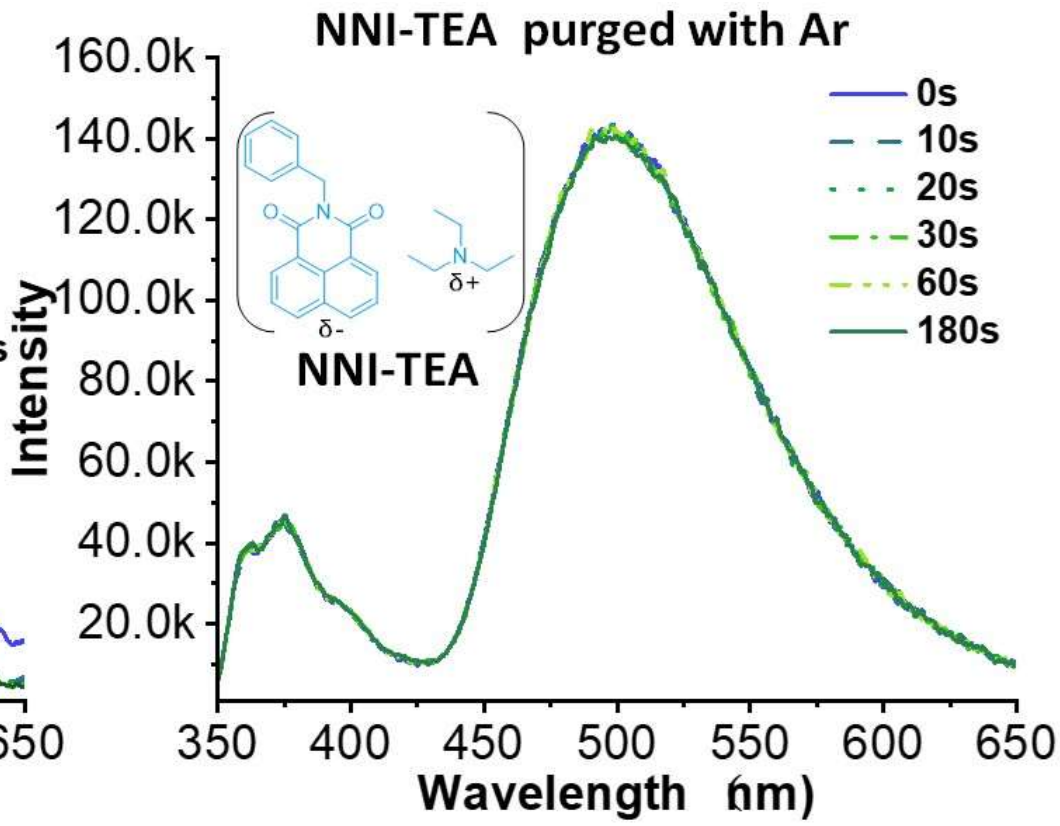


The PICTC formation and fluorescence is solvent sensitive: PICTC cannot form in methylbenzene (MB) since NNI forms an exciplex with MB. A Meisenheimer complex should not have been affected.

PICTC can be re-excited into a polar exciplex state by visible photon.

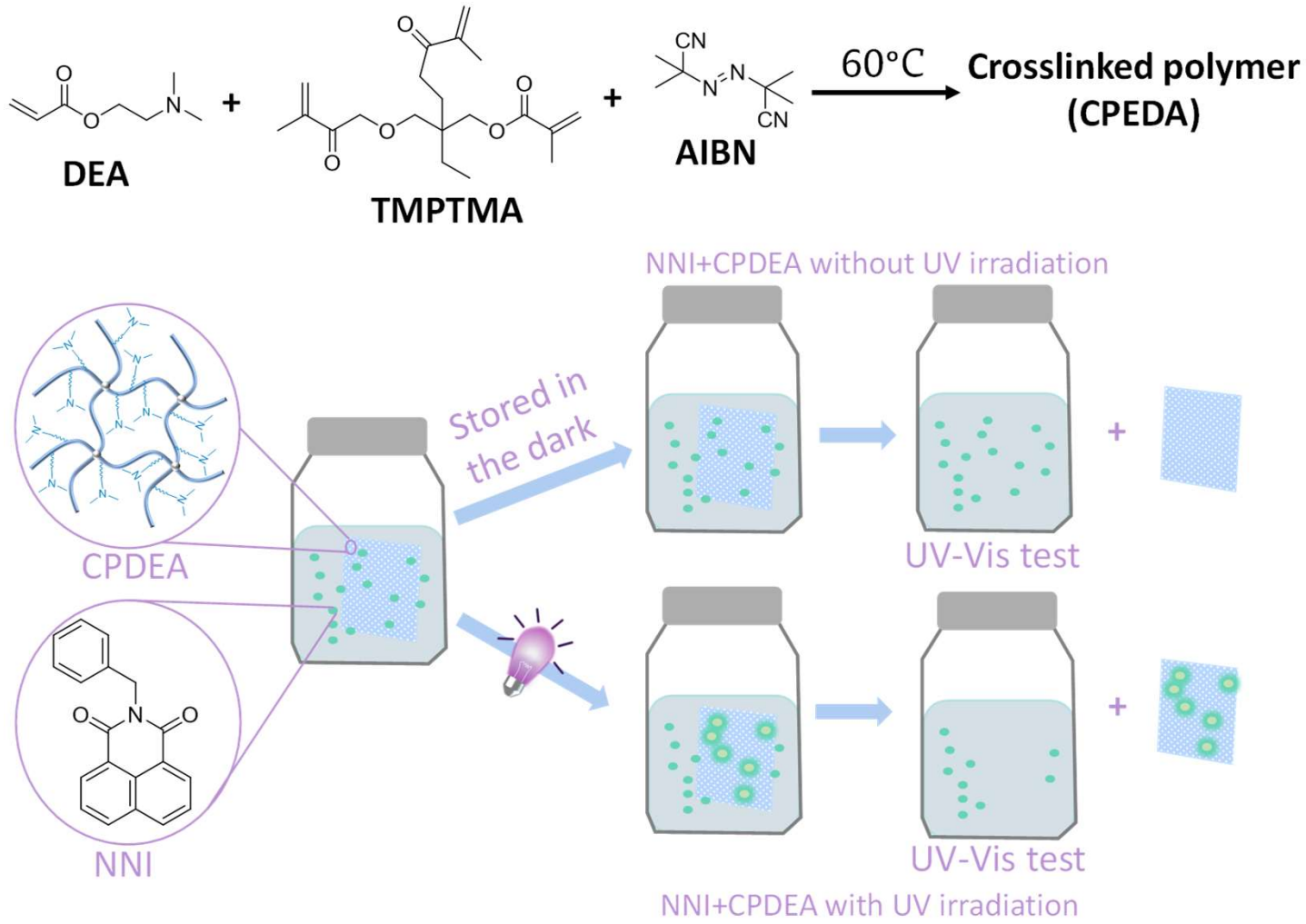
Reversible Destruction of PICTC by O_2



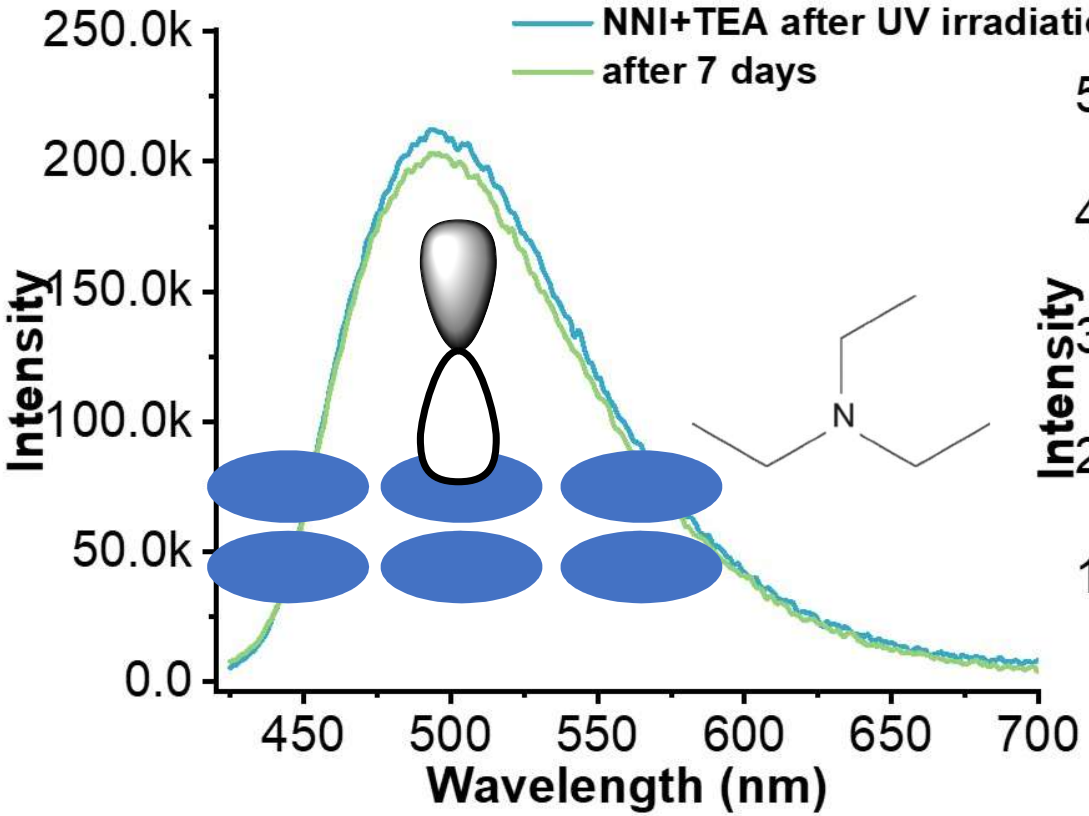


Air (both oxygen and CO_2) may induce disintegration of PICTC with the former being more quickly. A small percentage of PICTC is permanently oxidized.

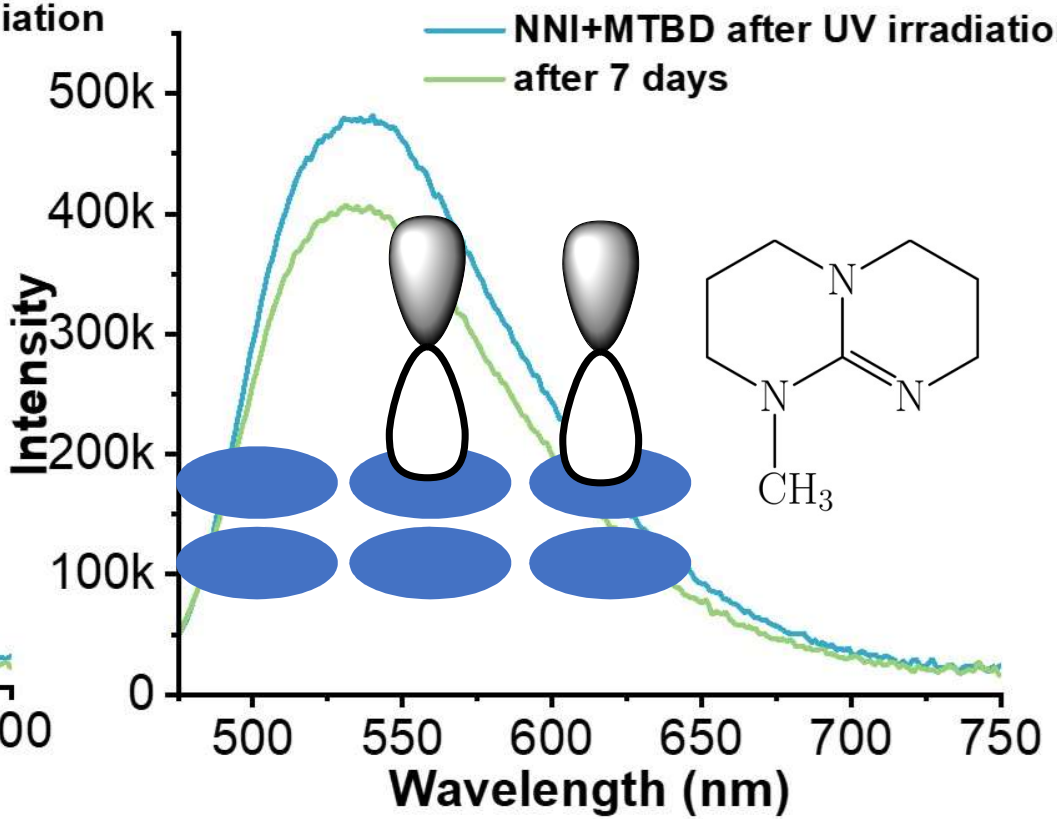
Sequestration by Light



A Deviation from Strict σ Donor

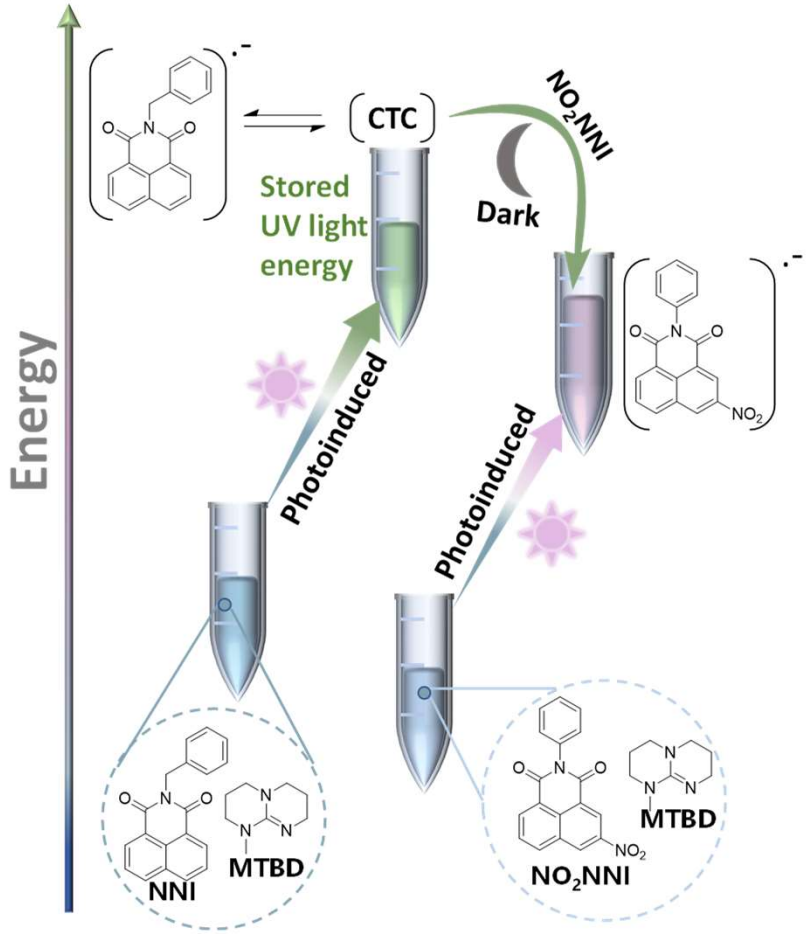


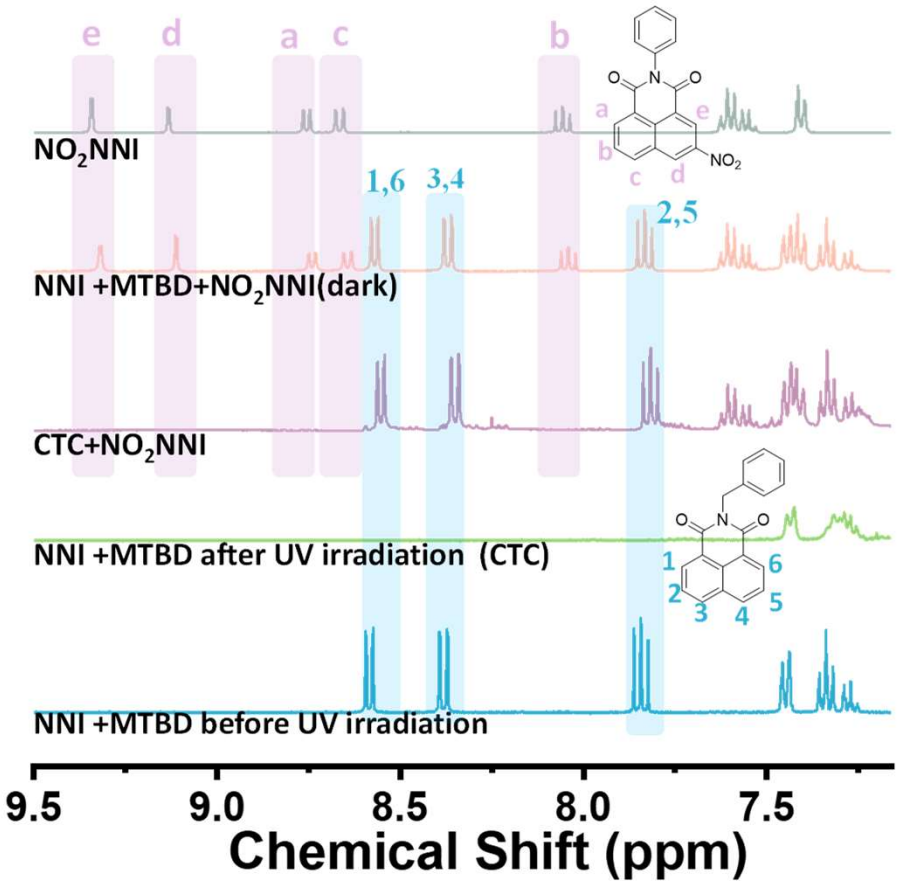
NMR Signal: Yes
EPR Signal: No



NMR Signal: No
EPR Signal: Yes

Application in Photochemistry





Acknowledgment



Dr. Wenhuan Huang (黄文环)

Funding from NSFC, USTC, MOST, and Anhui Kiwi Biotech Co. Limited

02

近代物理进展 · 专题报告 / MODERN PHYSICS PROGRESS

可信测量与复杂微环境动力学

RELIABLE MEASUREMENT AND COMPLEX MICROENVIRONMENTS

发光信号究竟来自谁？在手性、冰相与聚集体中，激子又走向哪里？

建议讲授 / Time 16 分钟

测量基准：ppb 级杂质也能主导高效室温磷光

Trace Impurities and a Noncrystalline-Solvent Standard

有机固体中，低于 10 ppb 摩尔比的客体掺杂即可产生明亮 RTP；量子产率可达 17.4%。

常规溶剂冷冻	微相分离	Dexter TTET	误判风险
二氯甲烷等发生微晶化	溶质与痕量杂质局部富集	主体三重态能量转移给杂质	杂质磷光被当作本征发光

新基准：使用低温下能玻璃化的非结晶介质，如 2-甲基四氢呋喃或无定形聚合物，阻断杂质敏化通道。

来源：申请书“主要学术成绩（二）”，第 7–8 页；Angew. Chem. Int. Ed. 2021, 60, 16970；2022, 61, e202206366。

手性匹配改变 Dexter 电子交换与能量转移速率

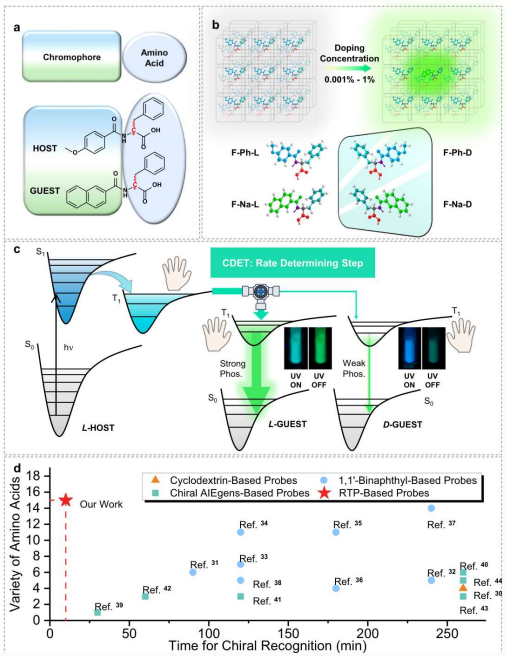
Chirality-Dependent Dexter Energy Transfer

手性匹配：三重态—三重态能量转移更高效

Chirality-dependent energy transfer / CDET

- 氨基酸转化为 F-Na-L / F-Na-D 手性能量受体。
- 掺入 F-Ph-L 主体纳米晶，敏化室温磷光。
- 同手性组合电子云重叠更有利，异手性组合响应较弱。

机制归属：短程 Dexter 电子交换，而非长程偶极 FRET。



五年报告图 65 | 手性 RTP 体系与 CDET 机制

来源：五年报告图 65；申请书第 8 页；Nat. Commun. 2023, 14, 1514。

从机制到通用识别：单一传感器区分 15 对氨基酸

Universal Chiral Readout of Amino Acids

25.8 倍

模型体系 L@L / D@L 磷光强度比

> 600 ms

模型体系 RTP 寿命

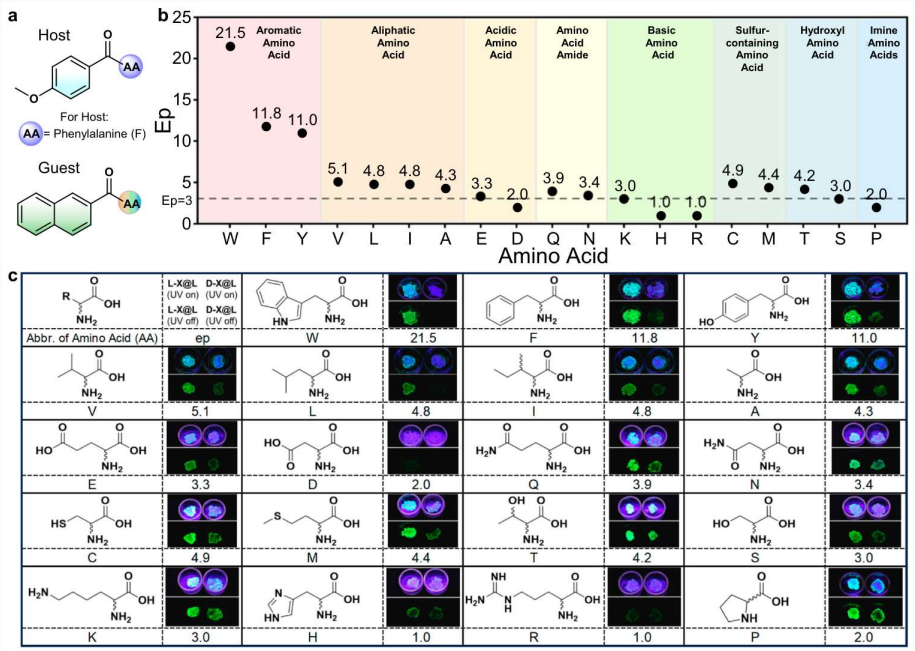
ep ≥ 3

全部 15 对均可可靠区分

21.5

色氨酸的最高 ep 值

识别流程压缩至数分钟；引入溴重原子可使 ep 提升 2 倍以上。



五年报告图 67 | 15 对天然氨基酸的通用识别

来源：张国庆《2026 年最终报告》，图 66–67；Nat. Commun. 2024, 15, 3314。

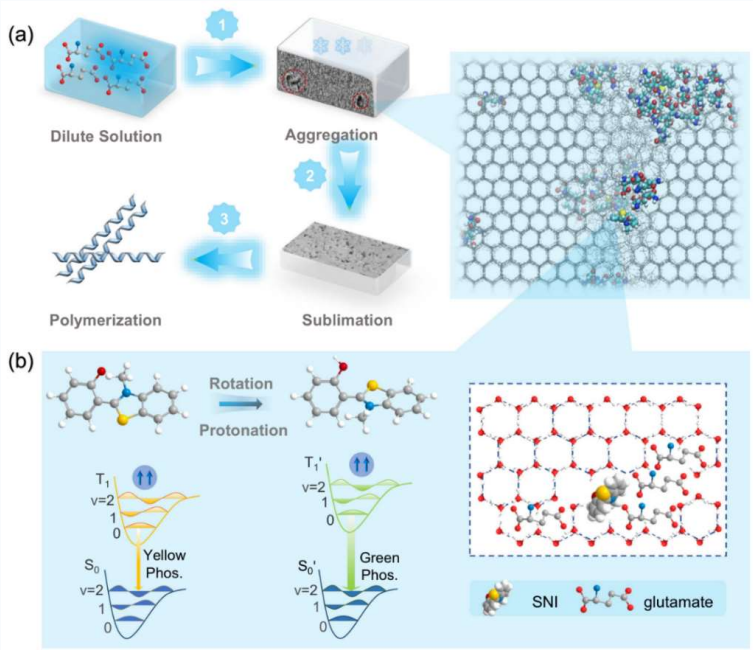
冰中氨基酸是否形成纳米聚集？用磷光原位读出

Phosphorescent Readout of Amino Acids in Ice

挑战：真实环境浓度低，吸收型技术难以直接读出冰中有机物的局域组织。

- SNI 含酚基给体与苯并噻唑鎓受体。
- 构象、质子化和氢键共同改变磷光。
- 77 K 水冰：磷光峰 597 nm，寿命 25.17 ms。

把“是否存在纳米聚集”转化为“光子态是否出现可判读差异”。



五年报告图 15 | SNI 探针与冰相聚集设想

来源：五年报告 2025 年冰相工作，图 15–16；Nat. Commun. 2025, 16, 10873。

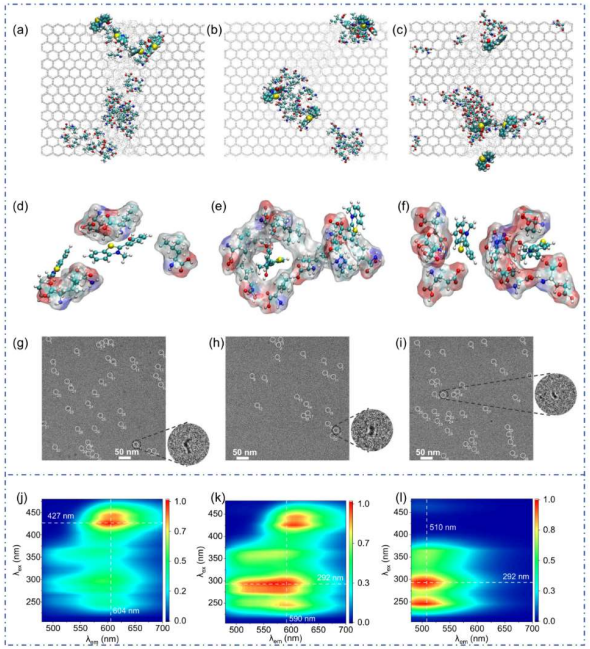
光谱—模拟—冷冻电镜：三种证据指向纳米聚集

Spectroscopy, Simulation and Cryo-TEM Evidence

光谱负责灵敏读出；模拟与电镜负责把光谱差异归因到结构。

- 亮氨酸：致密疏水团簇；冷冻电镜见约 3–5 nm × 5–20 nm 聚集体。
- 异亮氨酸缺陷更多；谷氨酸更延展、更亲水。
- 未加 SNI 的对照样品仍有 2–8 nm 聚集体，排除探针诱导。

峰位、颜色与寿命，成为聚集表面有序度和疏水性的光谱指纹。



五年报告图 17 | MD、静电势、冷冻电镜与二维磷光

来源：张国庆《2026 年最终报告》，图 16–17。

机制与边界：低温质子转移驱动微相分离

Low-Temperature Proton Transfer and Microphase Separation

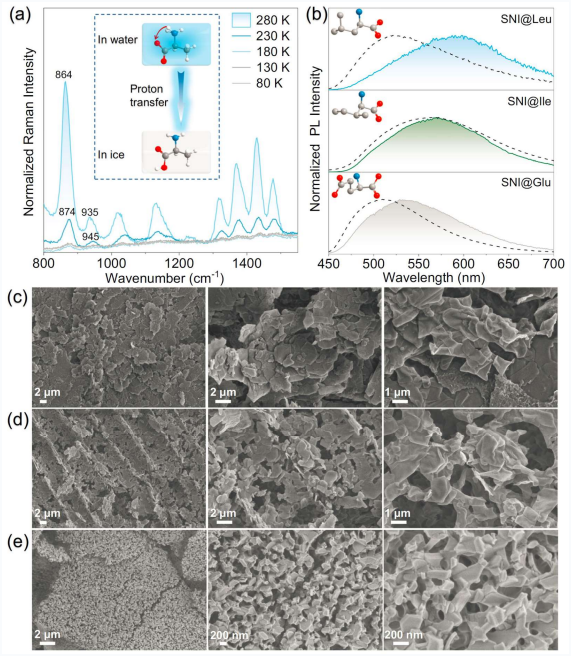
低温 水合稳定作用减弱

质子转移 丙氨酸拉曼峰约 180 K 突变

疏水性增强 驱动氨基酸纳米聚集

局部富集 为冰相前生物化学提供前提

SNI 去质子化：S_1/T_1 = 2.69/1.94 eV；质子化后升至 3.18/2.30 eV。



五年报告图 18｜变温拉曼、磷光与 SEM 对照

边界：证据支持冰相富集机制，但不等同于直接观测多肽形成。

来源：张国庆《2026 年最终报告》，图 18 与低温质子转移机制。

阶段小结 / Synthesis

可信构效关系，需要同时回答“来源、路径、环境”

From Spectral Signals to Reliable Structure–Property Relations

来源 / Origin	路径 / Pathway	环境 / Environment
本征分子还是痕量杂质?	FRET 还是 Dexter?	均相还是纳米聚集?
非结晶溶剂基准	手性匹配与动力学	光谱 + 模拟 + 电镜

有了可信测量，才能进一步把轨道、电场和聚集尺寸变成可预测的设计参数。

来源：依据申请书三项主要学术成绩归纳。

03

理性设计：轨道、电场与聚集体

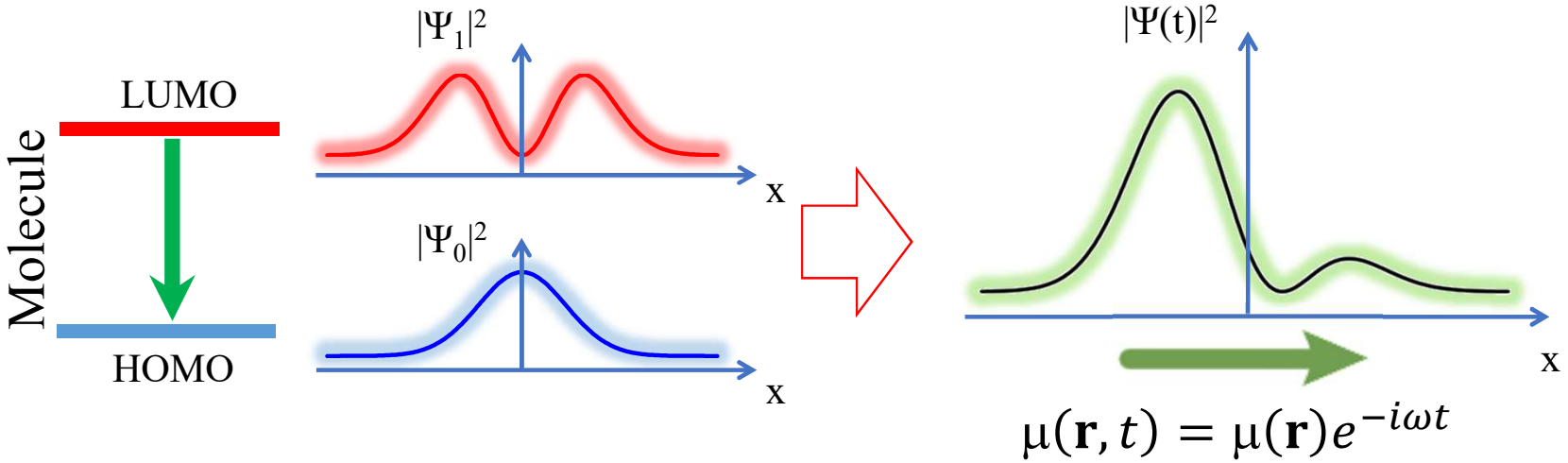
RATIONAL DESIGN: ORBITALS, FIELDS AND AGGREGATES

如何把机制理解转化为对反应性、ISC、寿命与发光通道的预测？

背景：跃迁偶极矩 (Transition Dipole Moment)

跃迁偶极矩 μ，在初态m与末态n间的跃迁过程里代表了两个态间跃迁的电偶极矩。跃迁偶极矩是一个含相因子的复矢量，它的方向代表跃迁的极性方向，振幅平方代表了由于系统内电荷分布导致的相互作用强度。

Molecular absorption/fluorescence → transition dipole moment



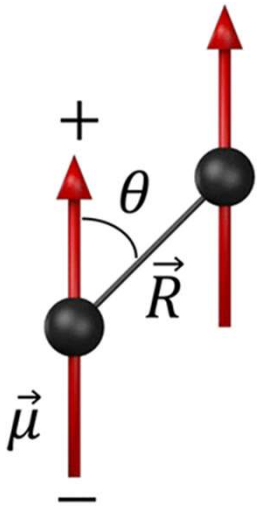
$$\mu(\mathbf{r},t) = \mu(\mathbf{r})e^{-i\omega t}$$

Animation Courtesy of 张杨

Kasha二聚体激子理论的量子相干性

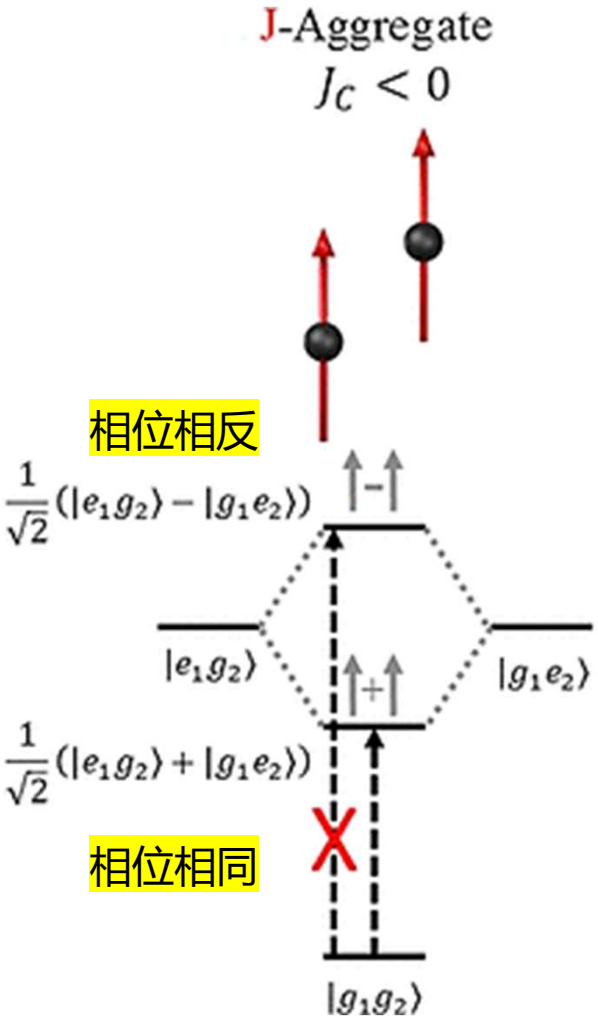
$$\Psi_{\mathrm{dim},e} = (\psi_{1,\mathrm{e}}\psi_{2,g} \pm \psi_{1,g}\psi_{2,e})/\sqrt{2}$$

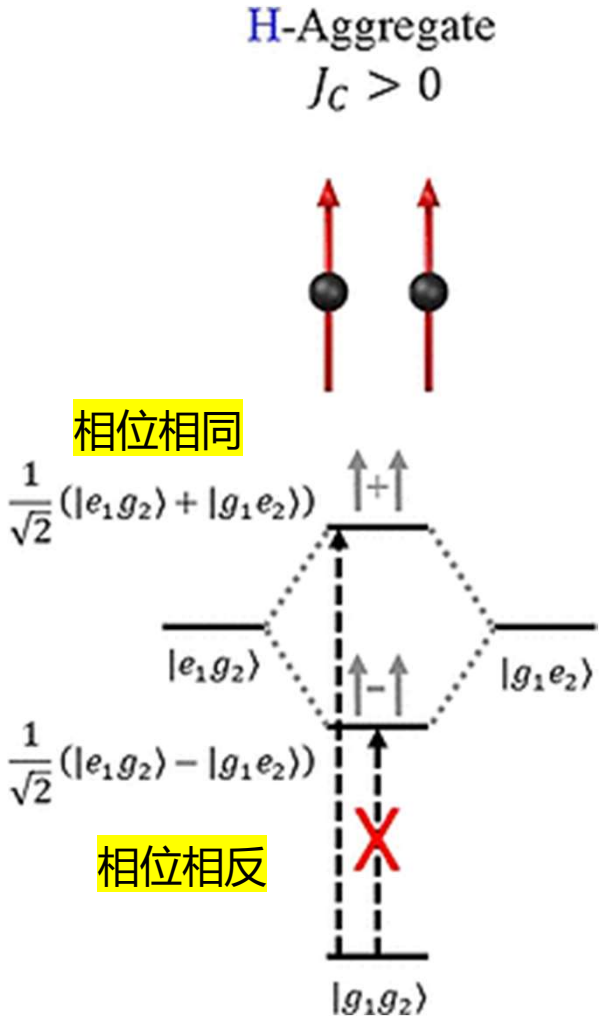
全同粒子



$$J_C^{pd} = \frac{\mu^2(1-3\cos^2\theta)}{4\pi\varepsilon R^3}$$

偶极-偶极





离散分子聚集体中的相干激子模型

$$H_{ex} = E_M + D + \sum_{m,n} J_{m,n}|m\rangle\langle n| \quad \Rightarrow \quad |k\rangle = \frac{1}{\sqrt{N}}\sum_n e^{ikn}|n\rangle \qquad k = 0, \pm 2\pi/N, \pm 4\pi/N, \ldots, \pi$$

$$\frac{1}{\sqrt{N}}\{ + + + + + + \}$$

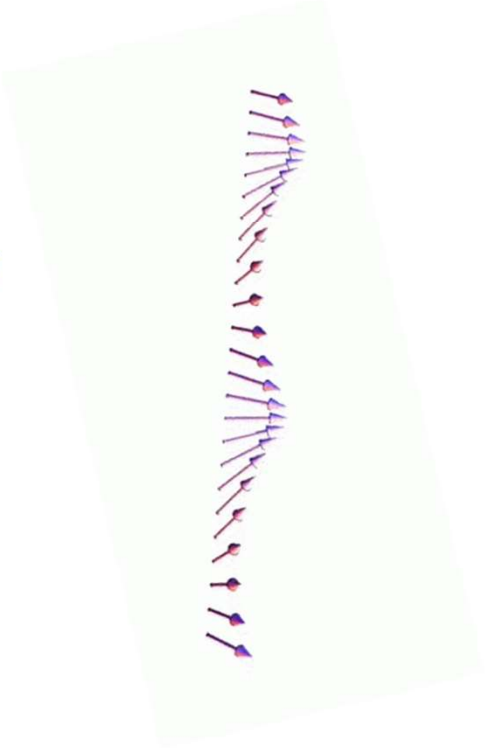
Aggregate transition dipole moment: $\langle G|\hat{\mu}|k=0\rangle = \sqrt{N}\mu_M$

$$|k=\pi\rangle = \frac{1}{\sqrt{N}}\sum_n (-1)^n |n\rangle$$

$$\frac{1}{\sqrt{N}}\{ - + - + - \}$$

$$\frac{1}{\sqrt{N}}\{ + + + + + + \}$$

$$\langle G|\hat{\mu}|k=\pi\rangle = 0$$



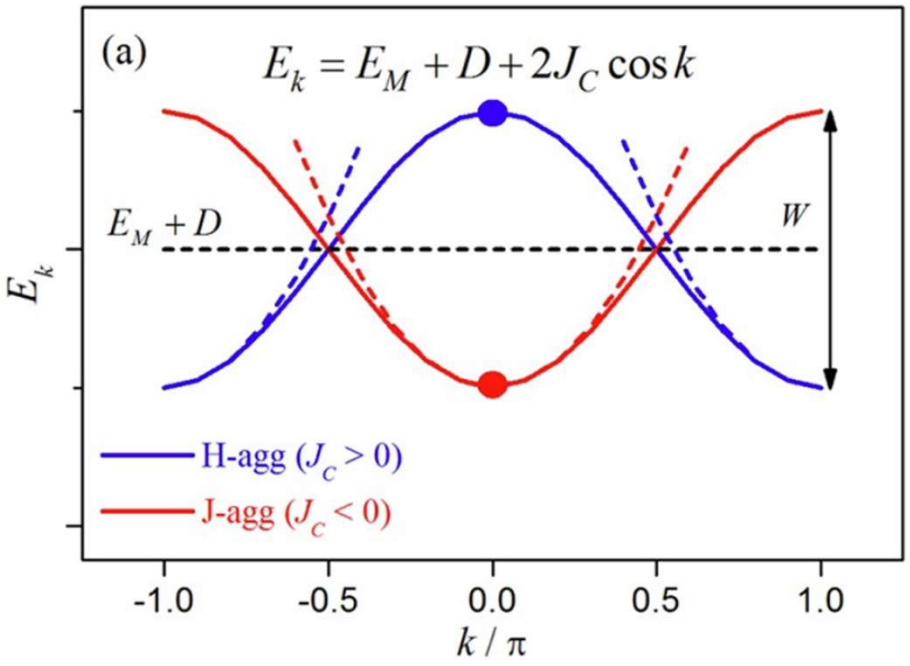
Chem. Rev. **2018**, 118, *15*, 7069-7163

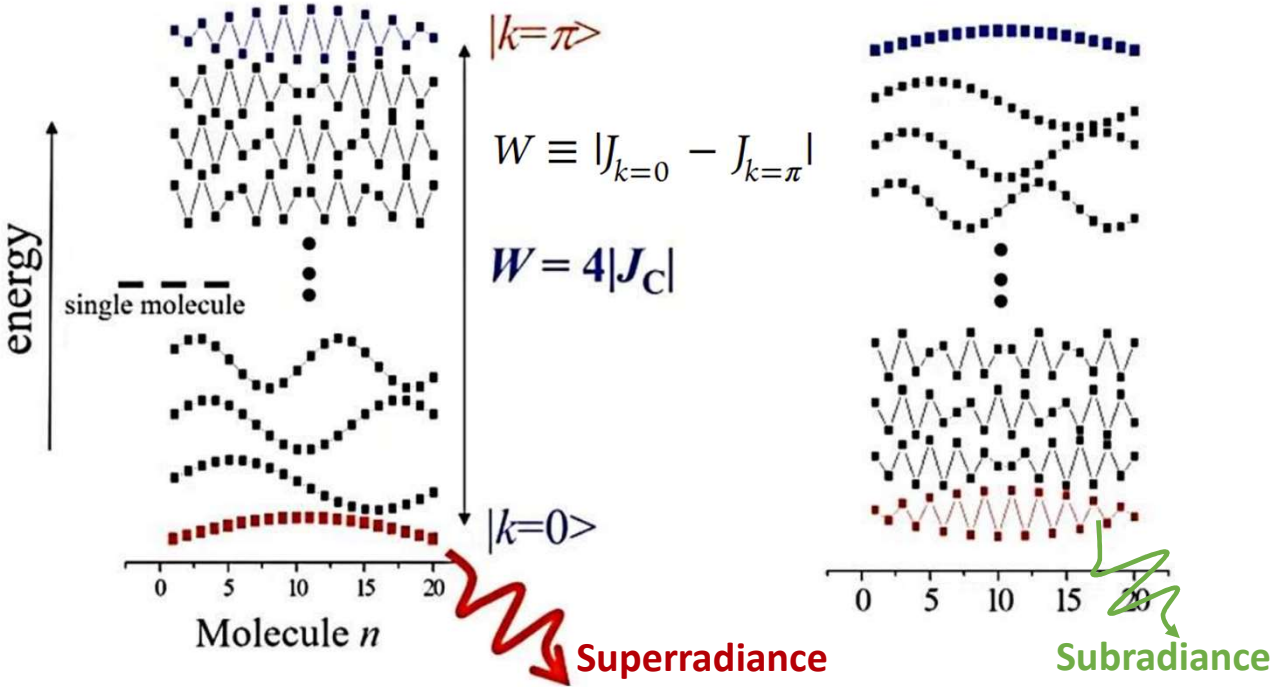
聚集体中不同的相干激子态 |k⟩

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_n e^{ikn}|n\rangle \quad k = 0, \pm 2\pi/N, \pm 4\pi/N, ..., \pi \qquad H_{ex} = E_M + D + \sum_{m,n} J_{m,n}|m\rangle\langle n|$$

不同的 ***k*** 值决定了分子之间不同的相位关系

$J_C < 0$: *J*-aggregates　　$J_C > 0$: *H*-aggregates



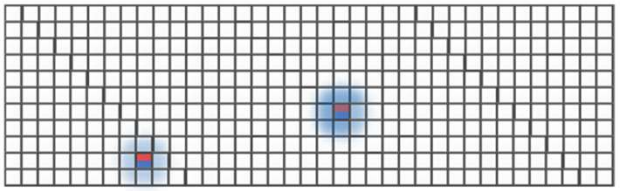


具有量子相干性的聚集体激子传能是否更加高效?

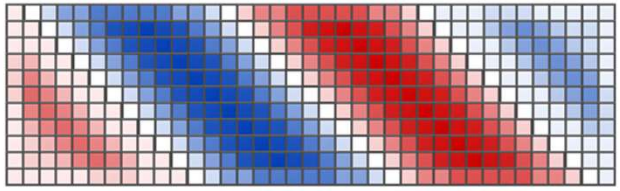


谌旎宇博士
现华为工程师

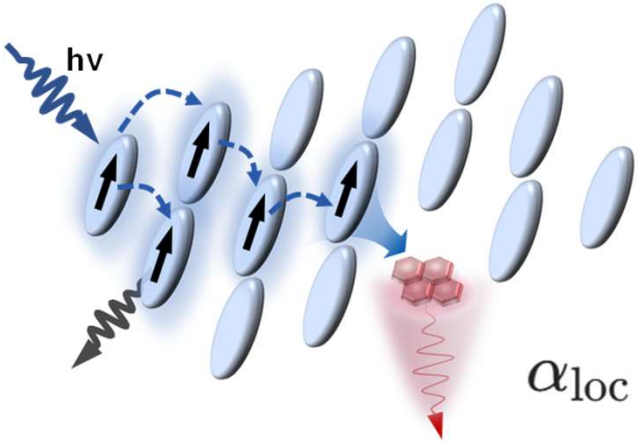
迄今为止没有直接实验证据



相空间

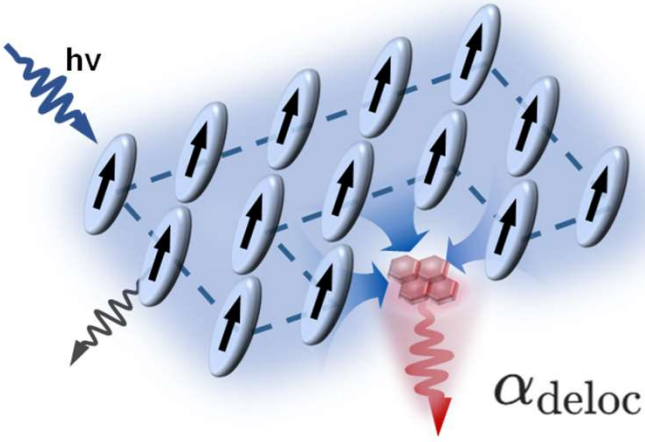


$$\frac{dN_A^*}{dt} = \alpha N_D^*$$



Under-Sensitized Host Luminescence

实空间



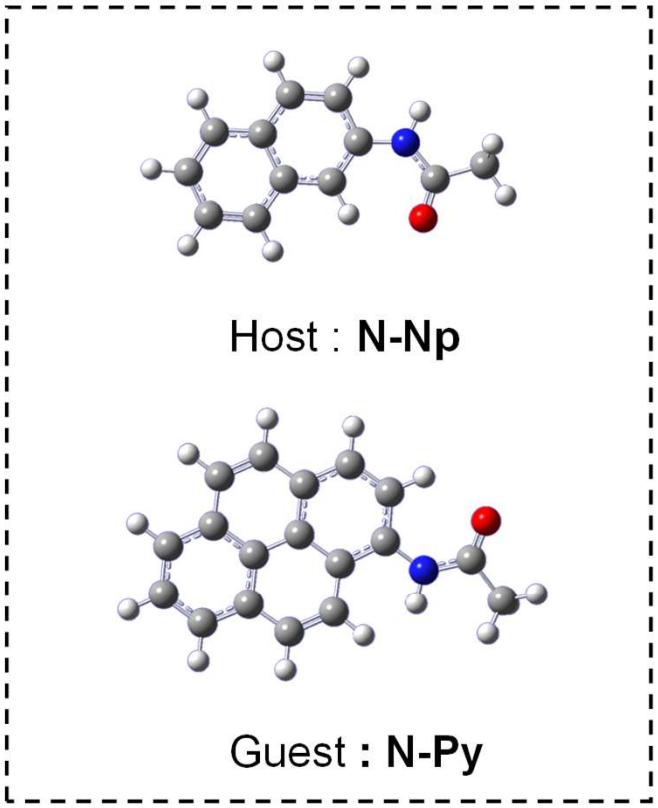
Hyper-Sensitized Host Luminescence

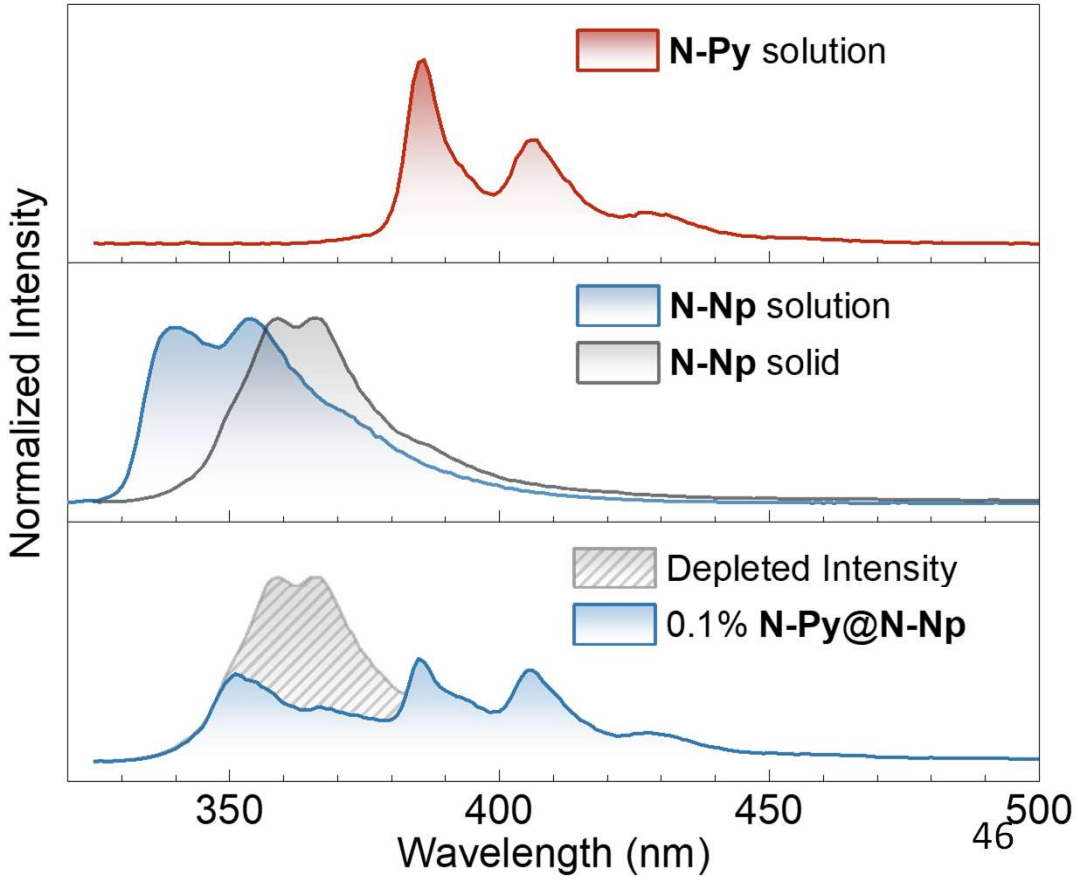
$$\begin{aligned}
\alpha_{\mathrm{deloc}} &\propto \left|\langle A_\beta | H_{DA} | D_\alpha \rangle\right|^2 \\
&= \left|\sum_{j,k} c_{\alpha j} c_{\beta k}^* V_{jk}^{DA}\right|^2 \\
&\leq \left|\sum_{j,k} \frac{1}{\sqrt{N_D}} \frac{1}{\sqrt{N_A}} V_{jk}^{DA}\right|^2 \\
&= N_D N_A \alpha_{\mathrm{loc}}
\end{aligned}$$

Chen, X.; Cheng, A.; et al. Huang, W.*; Zhang, G.* Probing Coherent Aggregate Exciton Energy Transfer in Organic Dopant Systems. *Sci. Adv., Under Review*

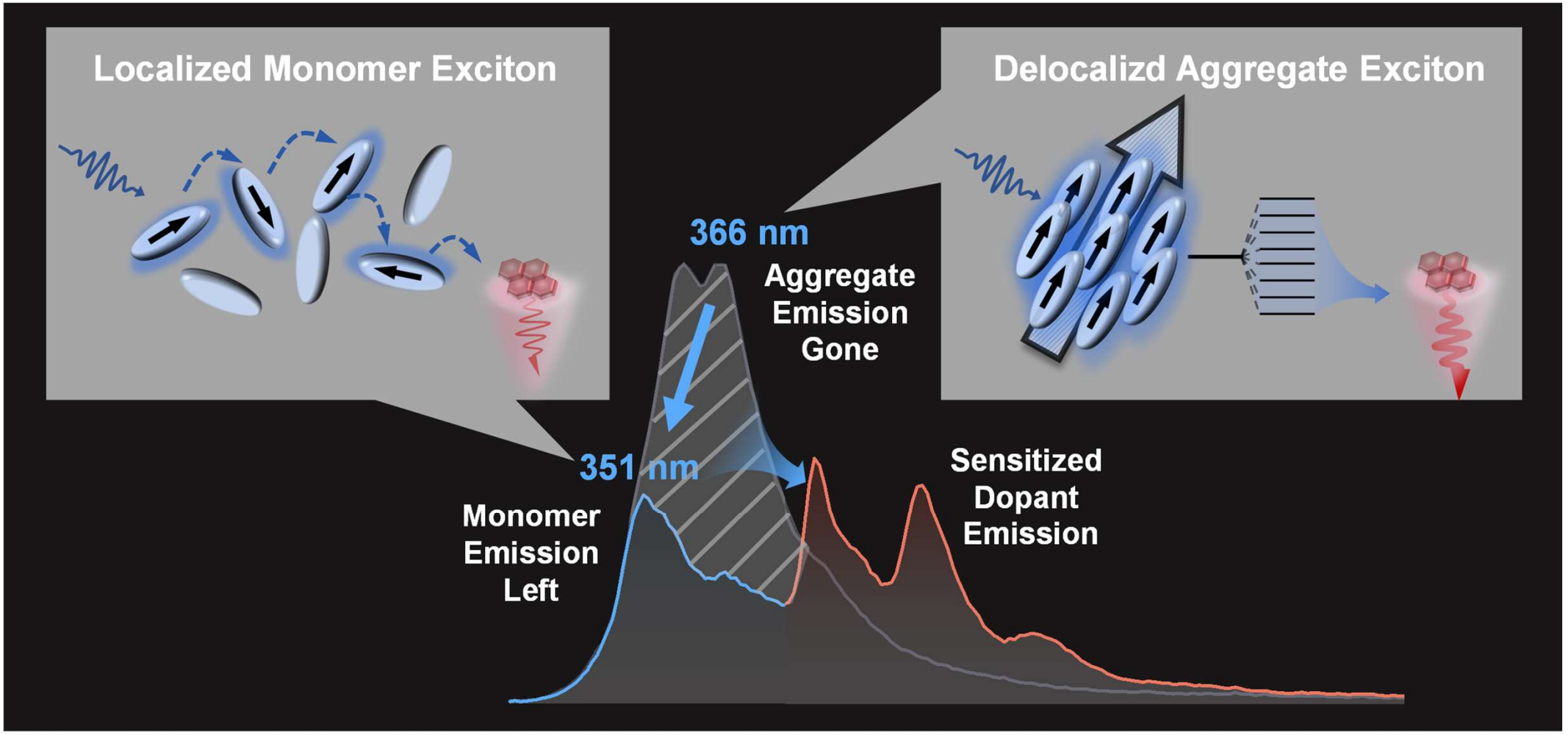
模型分子体系的选择和主要结论

能量给体：N-乙酰基氨基萘 能量受体：N-乙酰基氨基芘

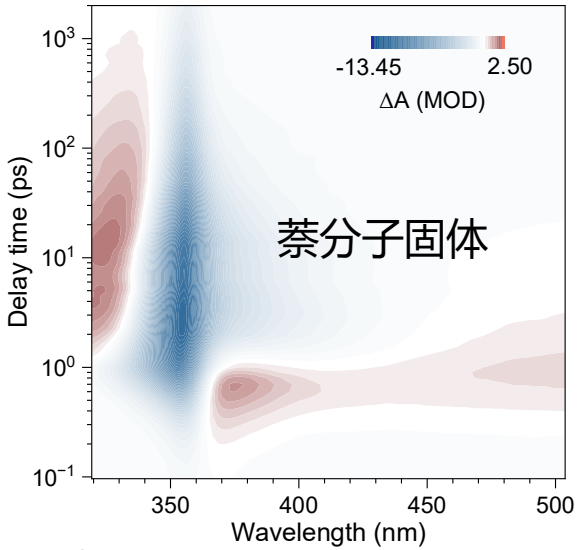


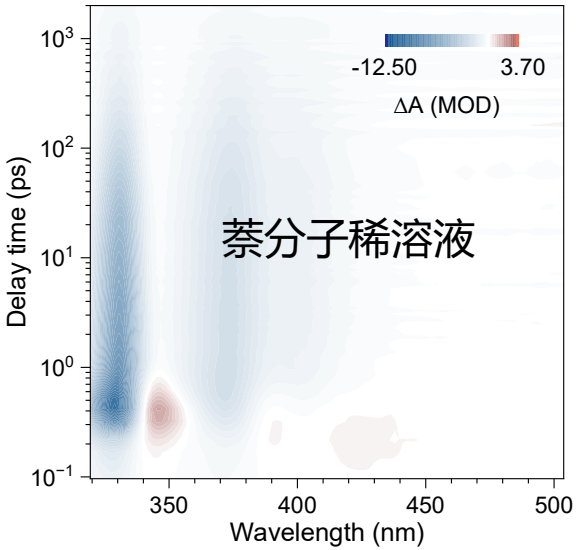


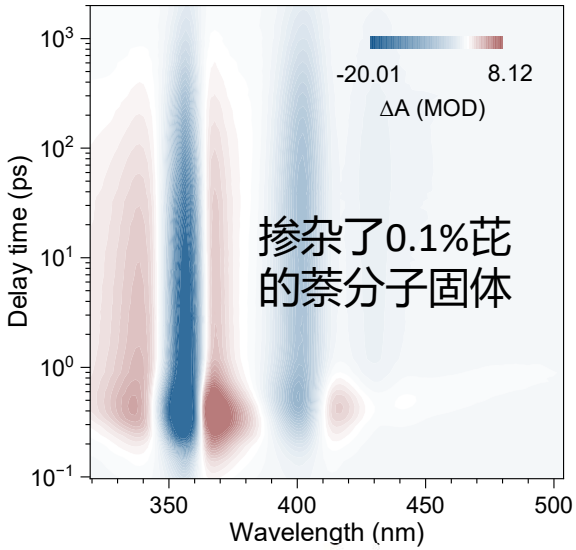
模型分子体系的选择和主要结论

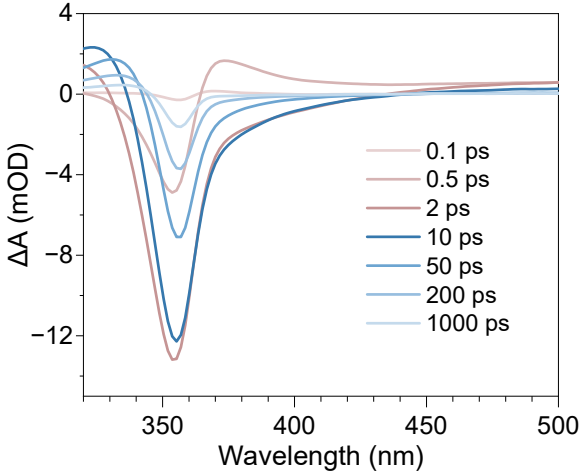


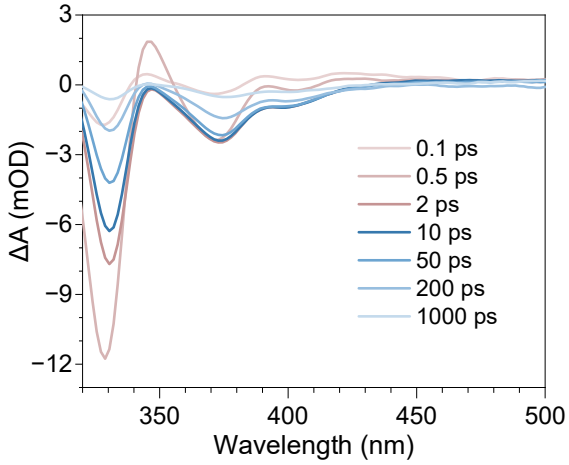
用能量受体掺杂前后超快吸收谱上的变化

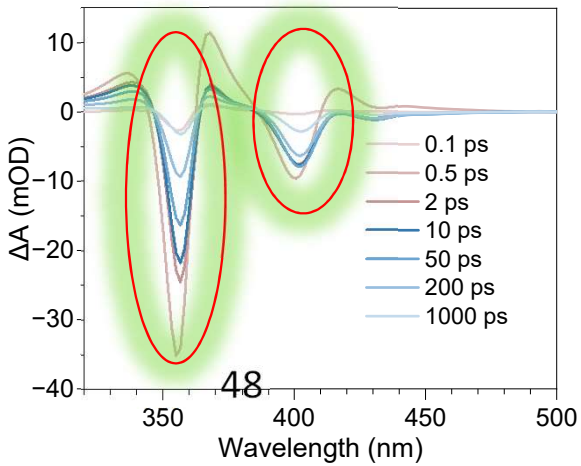


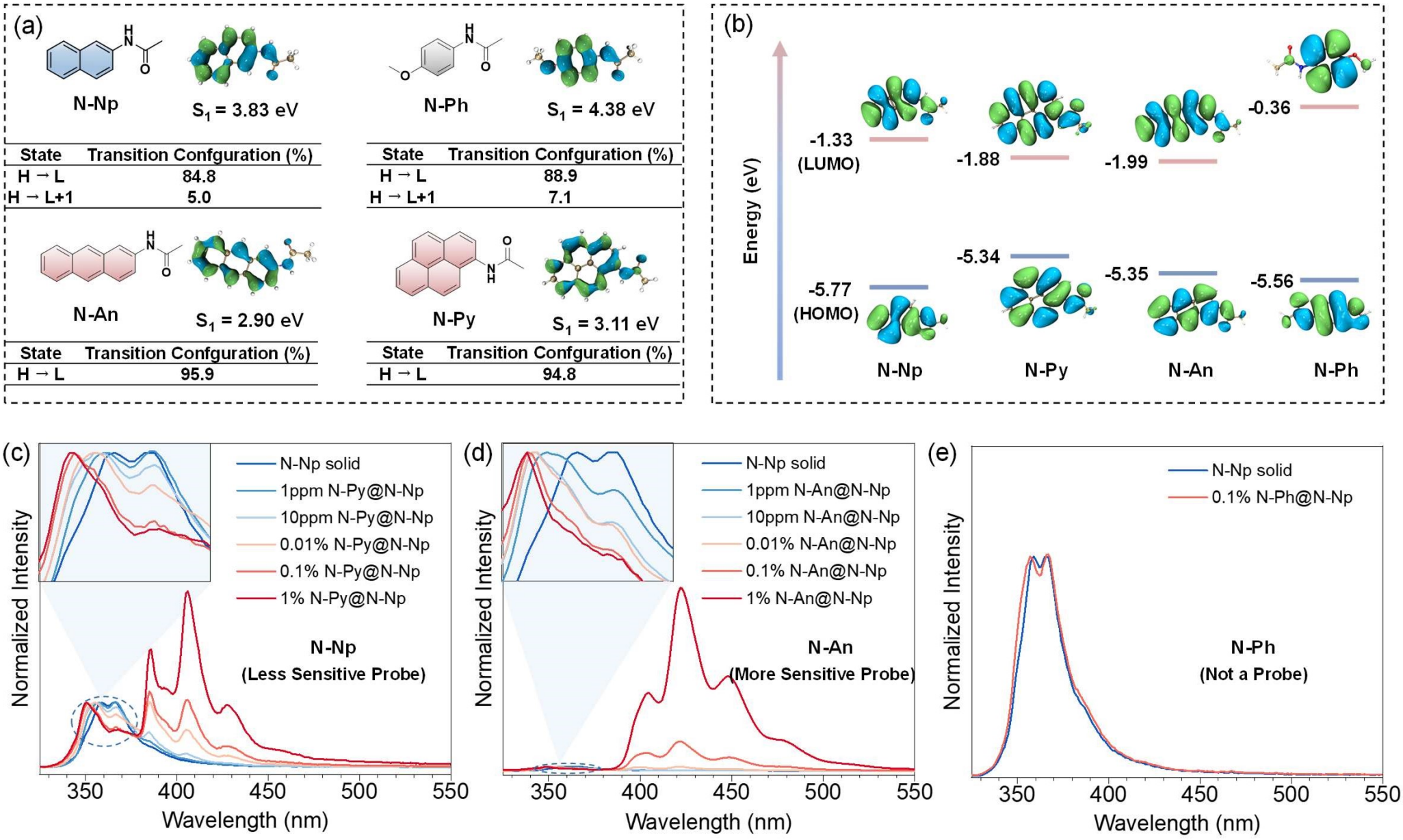


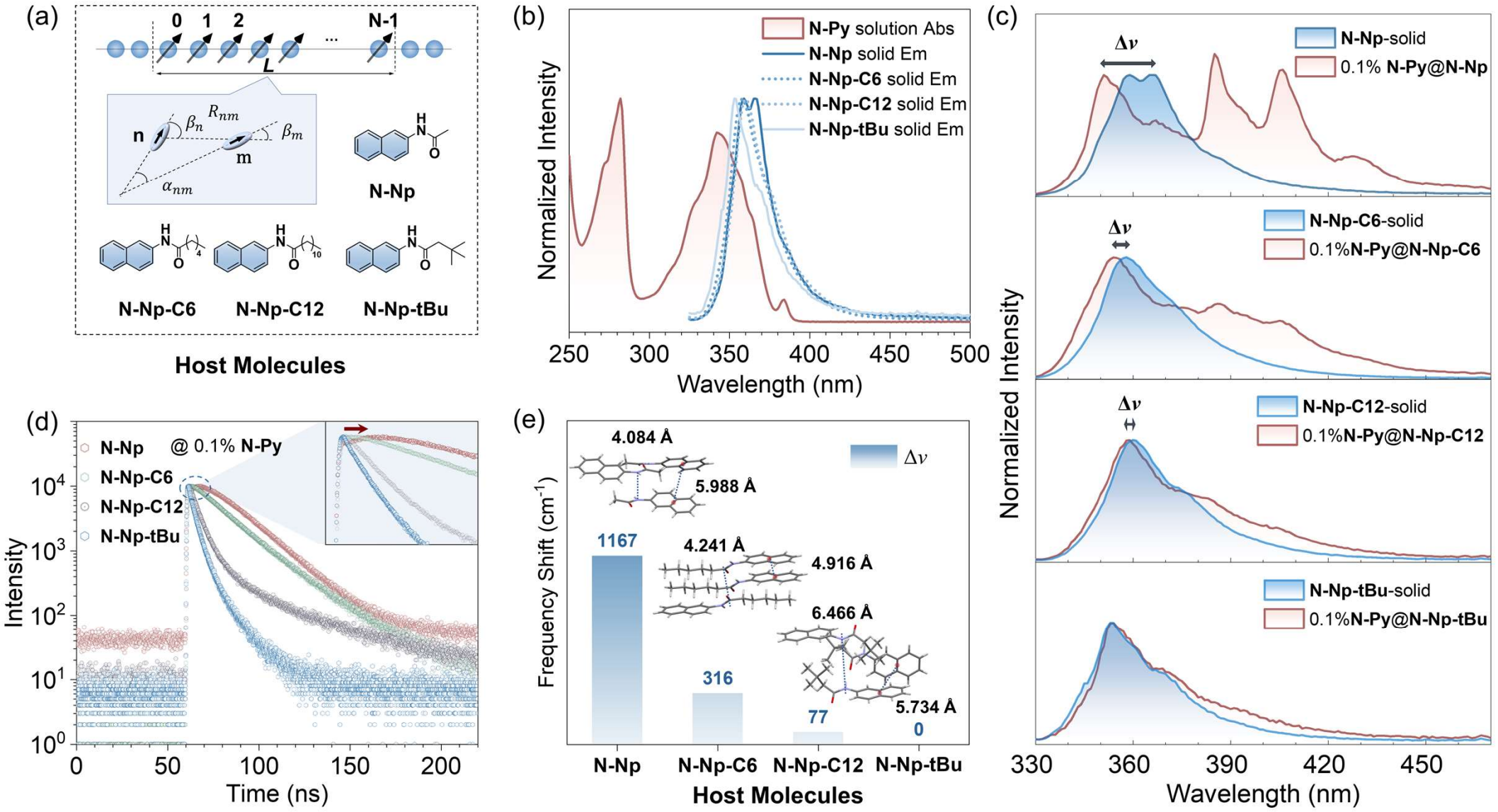








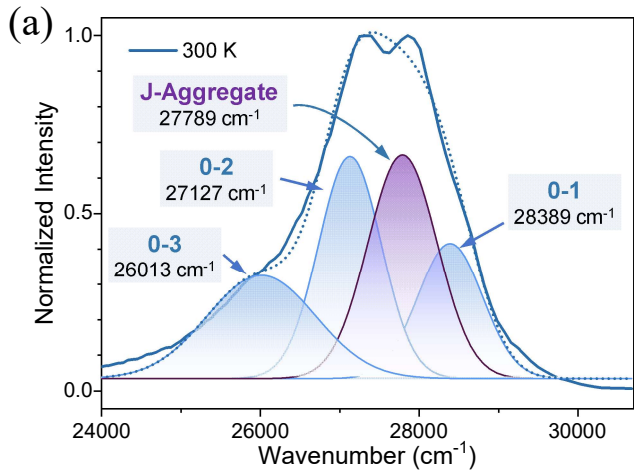

(a)
N-Np
S1 = 3.83 eV
State Transition Confguration (%)
H → L 84.8
H → L+1 5.0
N-Ph
S1 = 4.38 eV
State Transition Confguration (%)
H → L 88.9
H → L+1 7.1
N-An
S1 = 2.90 eV
State Transition Confguration (%)
H → L 95.9
N-Py
S1 = 3.11 eV
State Transition Confguration (%)
H → L 94.8
(b)
Energy (eV)
-1.33
(LUMO)
-1.88
-1.99
-0.36
-5.77
(HOMO)
-5.34
-5.35
-5.56
N-Np
N-Py
N-An
N-Ph
(c)
N-Np solid
1ppm N-Py@N-Np
10ppm N-Py@N-Np
0.01% N-Py@N-Np
0.1% N-Py@N-Np
1% N-Py@N-Np
N-Np
(Less Sensitive Probe)
Normalized Intensity
Wavelength (nm)
(d)
N-Np solid
1ppm N-An@N-Np
10ppm N-An@N-Np
0.01% N-An@N-Np
0.1% N-An@N-Np
1% N-An@N-Np
N-An
(More Sensitive Probe)
Normalized Intensity
Wavelength (nm)
(e)
N-Np solid
0.1% N-Ph@N-Np
N-Ph
(Not a Probe)
Normalized Intensity
Wavelength (nm)

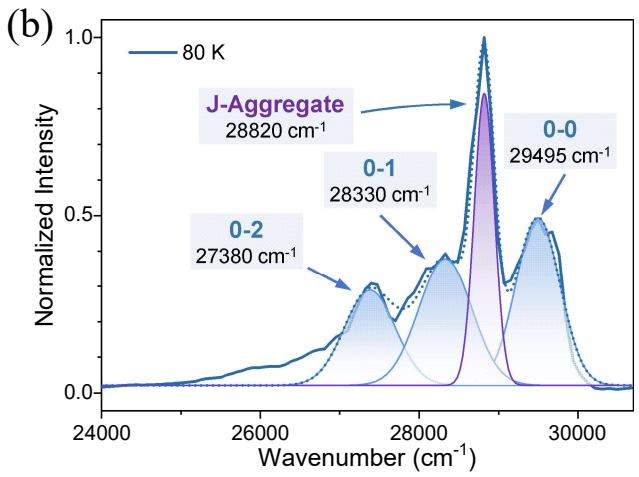

(a)
0 1 2 ... N-1
L
n
m
R_{nm}
β_n
β_m
α_{nm}
N-Np
N-Np-C6
N-Np-C12
N-Np-tBu
Host Molecules
(b)
N-Py solution Abs
N-Np solid Em
N-Np-C6 solid Em
N-Np-C12 solid Em
N-Np-tBu solid Em
Normalized Intensity
250 300 350 400 450 500
Wavelength (nm)
(c)
Δv
N-Np-solid
0.1% N-Py@N-Np
N-Np-C6-solid
0.1%N-Py@N-Np-C6
N-Np-C12-solid
0.1%N-Py@N-Np-C12
N-Np-tBu-solid
0.1%N-Py@N-Np-tBu
Normalized Intensity
330 360 390 420 450
Wavelength (nm)
(d)
N-Np @ 0.1% N-Py
N-Np-C6
N-Np-C12
N-Np-tBu
Intensity
10^4 10^3 10^2 10^1 10^0
0 50 100 150 200
Time (ns)
(e)
4.084 Å
5.988 Å
Δv
1167
4.241 Å
4.916 Å
6.466 Å
316
77
5.734 Å
0
Frequency Shift (cm^{-1})
N-Np N-Np-C6 N-Np-C12 N-Np-tBu
Host Molecules

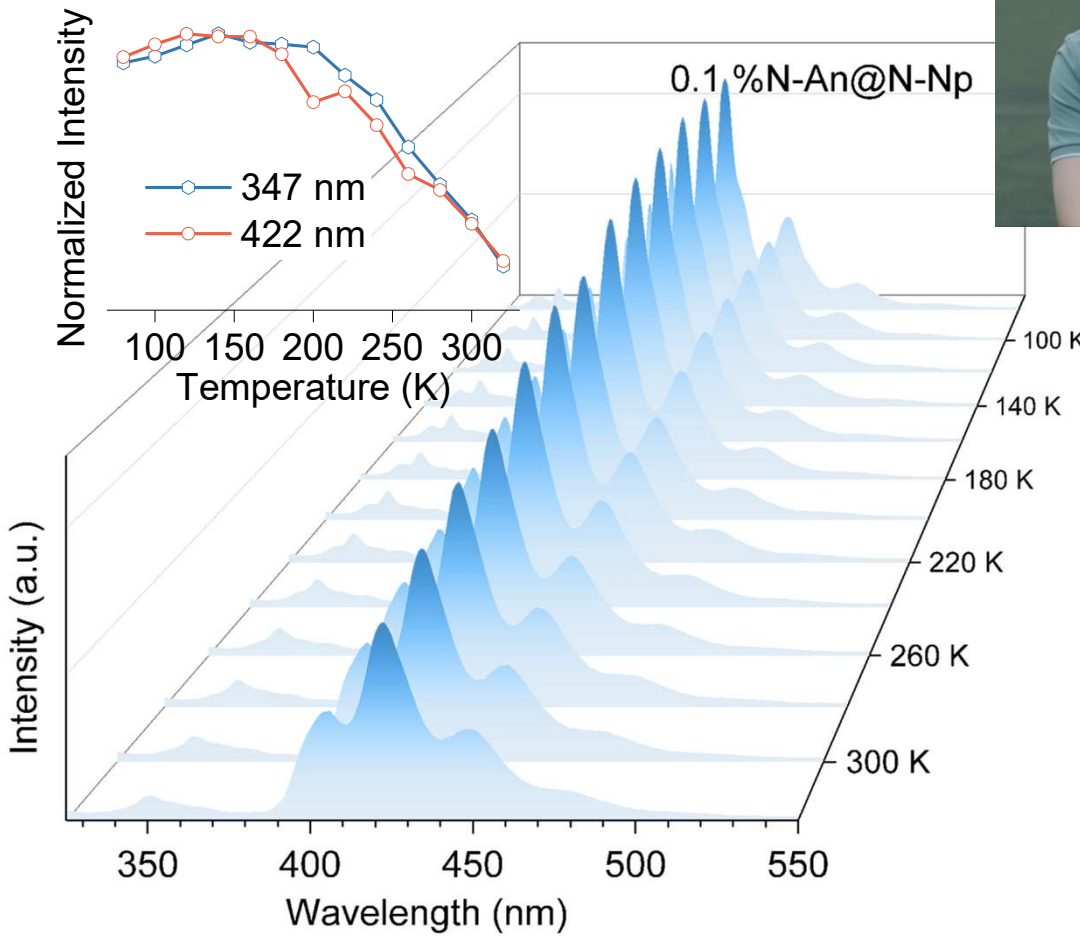
什么类型的聚集体在更高效的传递激子能量?



程奥远
博士生

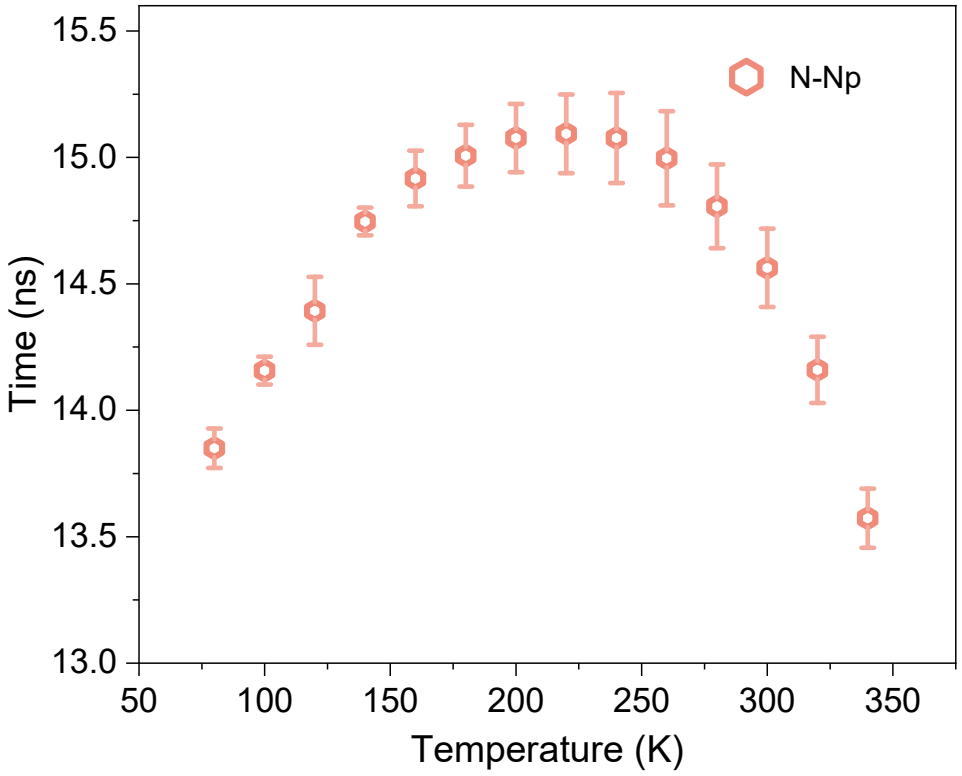


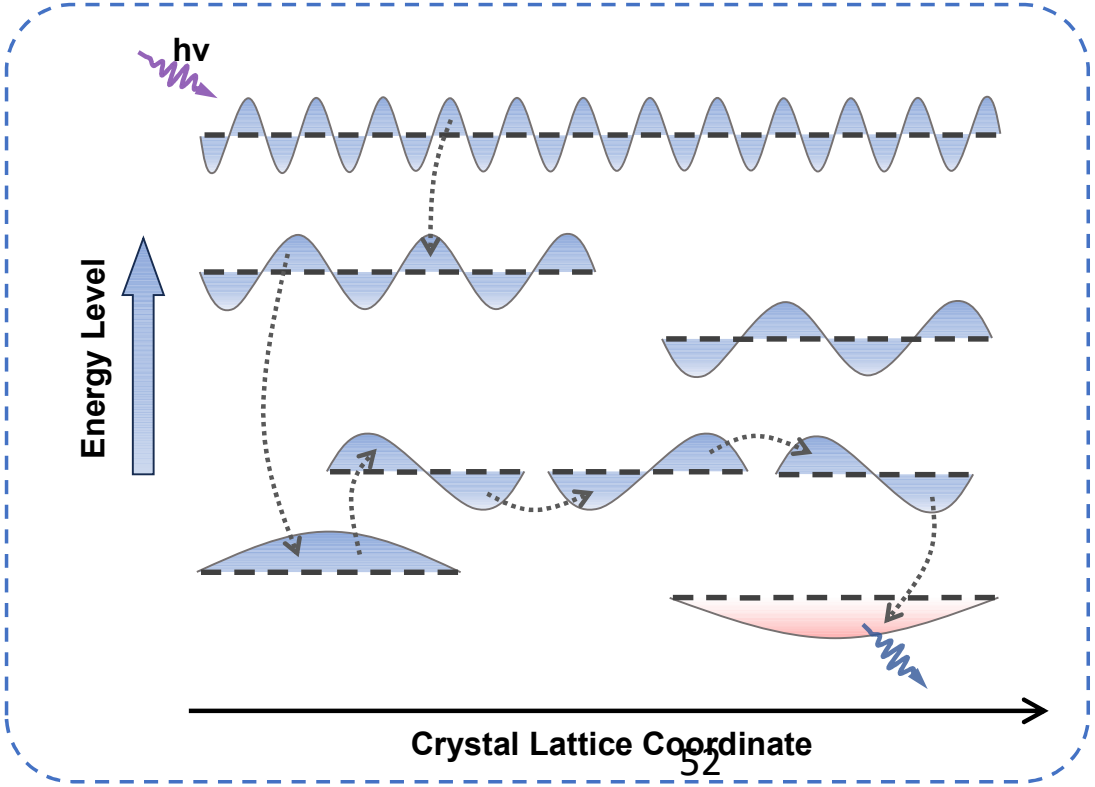




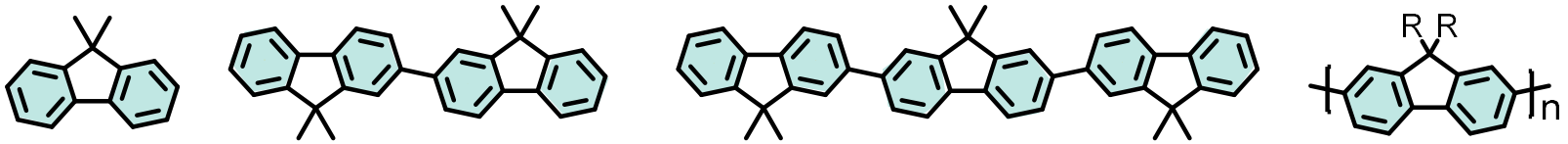
什么类型的聚集体在更高效的传递激子能量?

萘的固体随着温度升高，荧光寿命先增加后减小，在200K附近反转

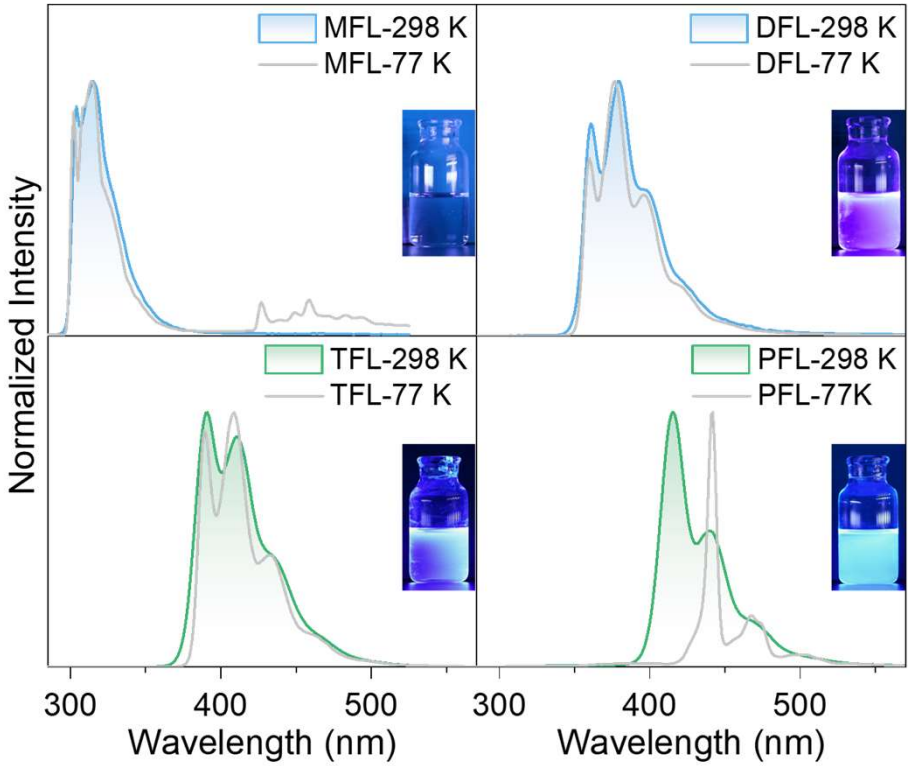




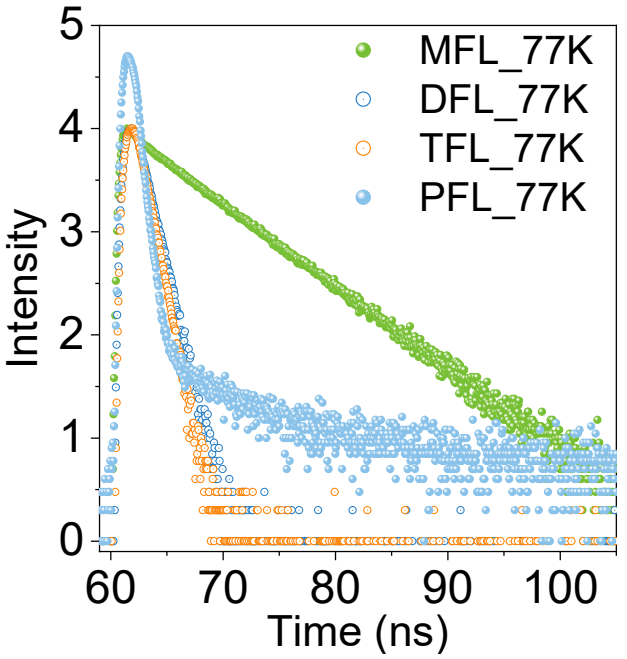
PFO蓝光PLED容易降解变绿问题



MFL DFL TFL PFL



$$H_{FH} = E_M + D + \sum_{m,n} J_{m,n}|m\rangle\langle n| + \omega_{vib}\sum_n b_n^\dagger b_n + \omega_{vib}\sum_n\{\lambda(b_n^\dagger + b_n) + \lambda^2\}|n\rangle\langle n|$$



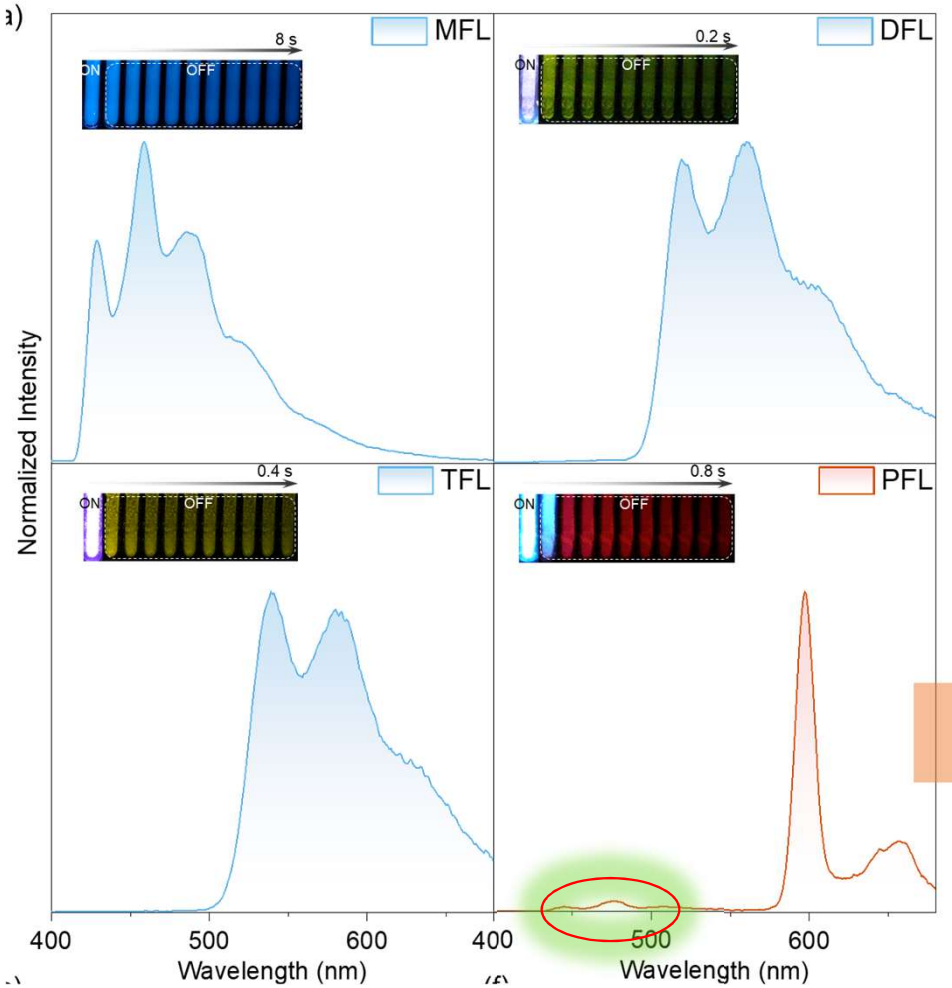


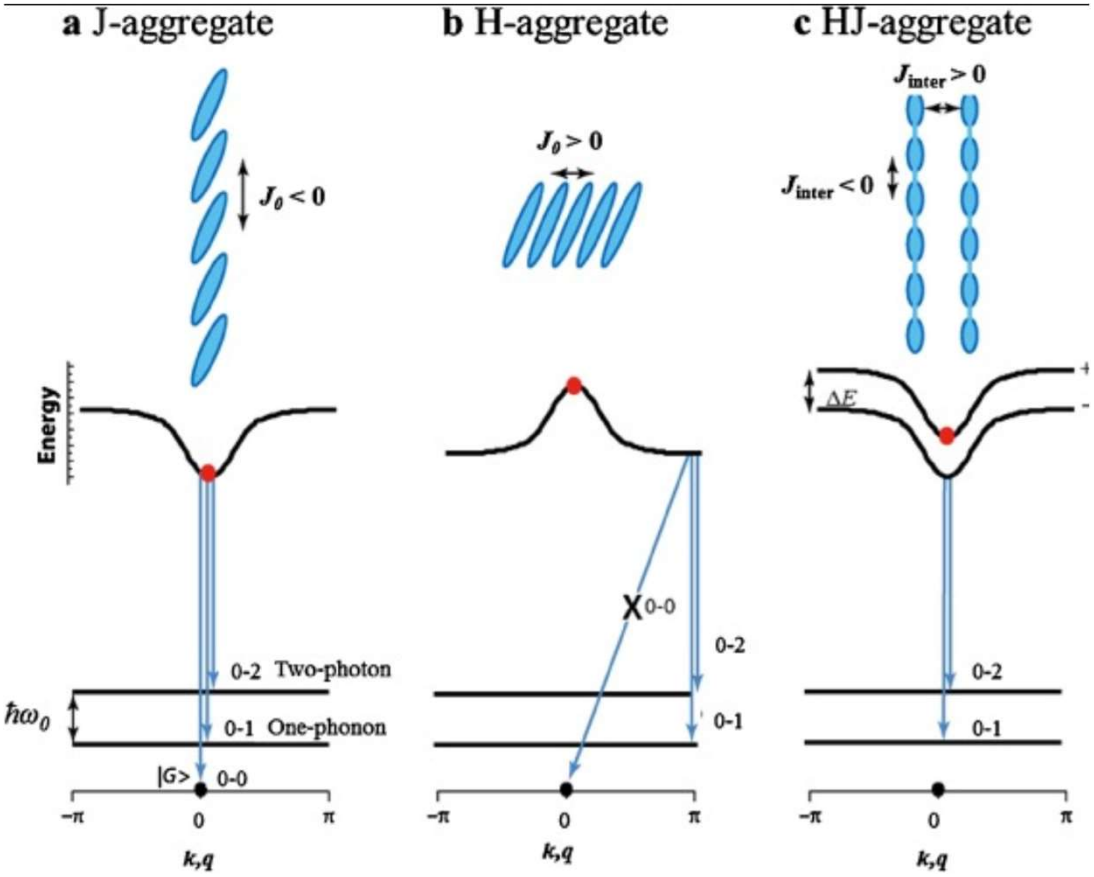
程光謇
博士生



刘洪平
博士生

反常的PFL磷光光谱：HJ-聚集体的形成

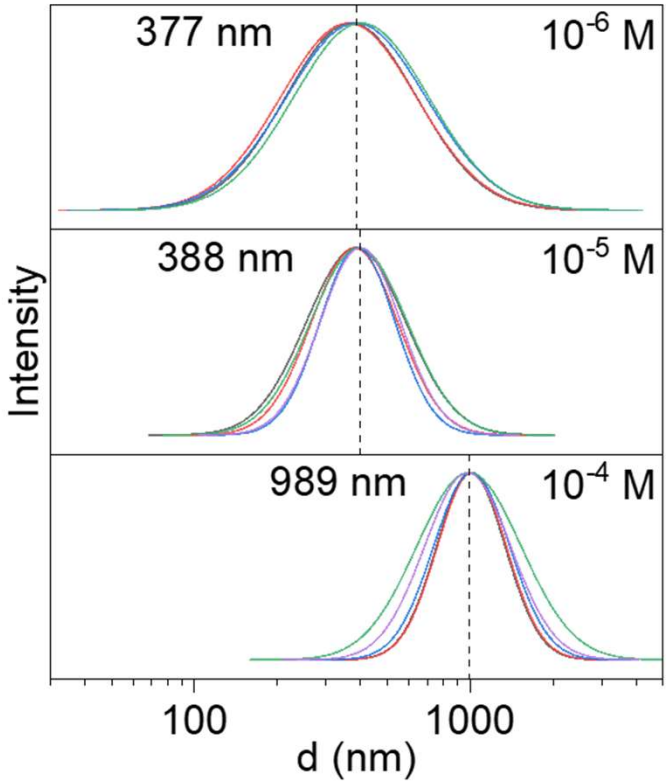


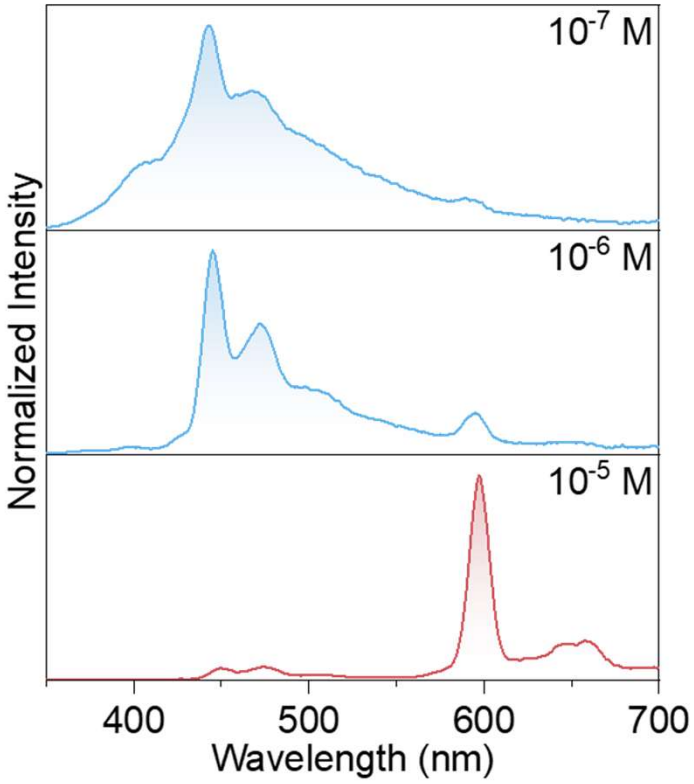


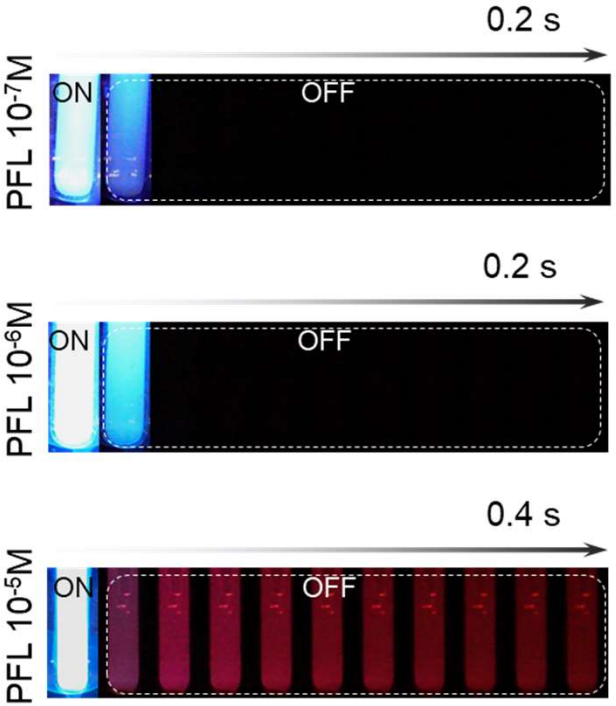
Tay-Agbozo, S.; Street, S.; Kispert, L. D. The Carotenoid Bixin: Optical Studies of Aggregation in Polar/Water Solvents. *J. Photochem. Photobiol., A* **2018**, *362*, 31–39.

聚集体尺寸依赖的激子发射

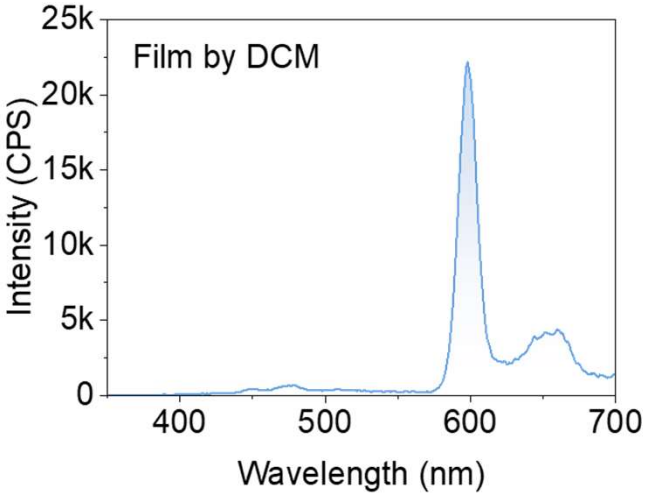
随着聚芴高分子的浓度增加，TTA逐渐变为相干激子的磷光发射

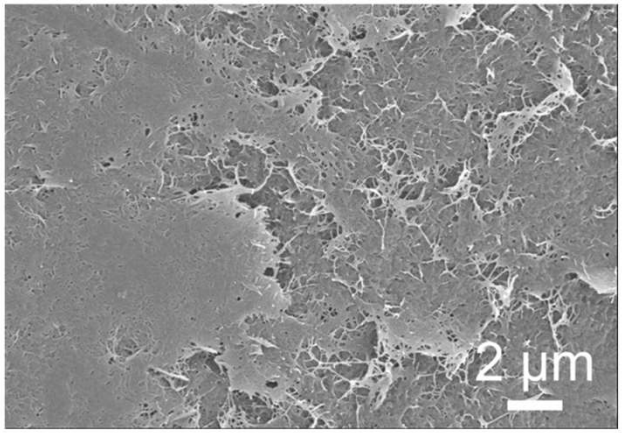


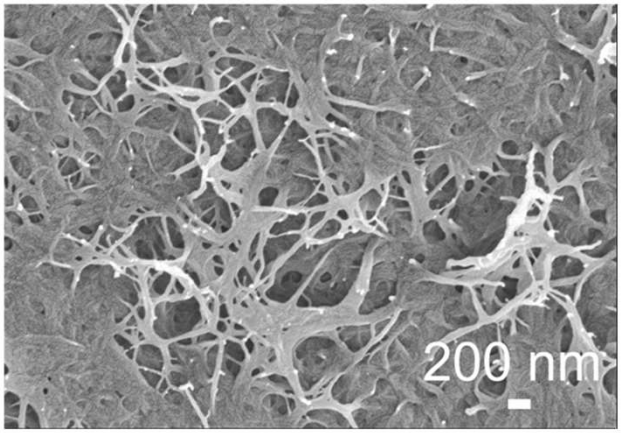


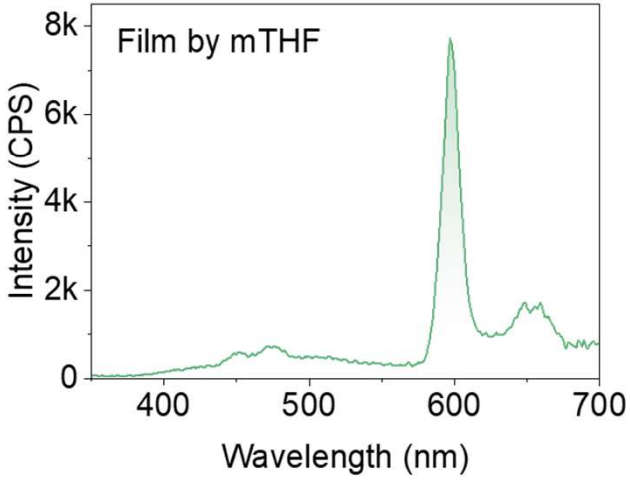


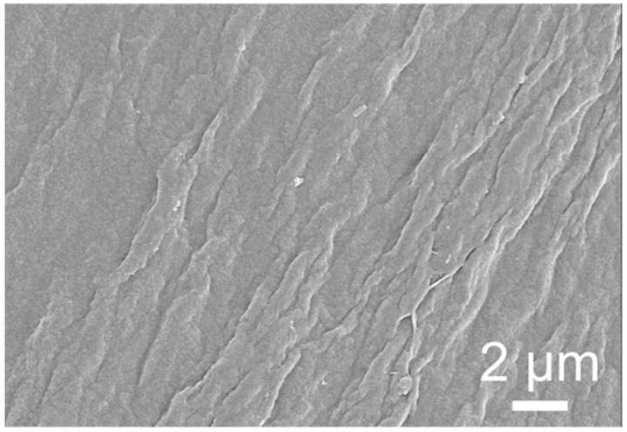
聚集体形貌依赖的激子发射

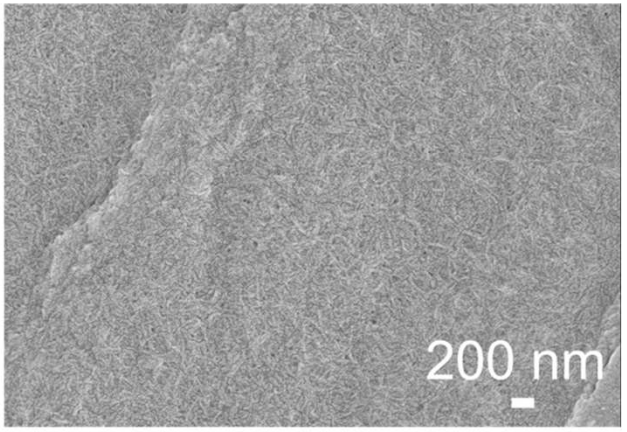






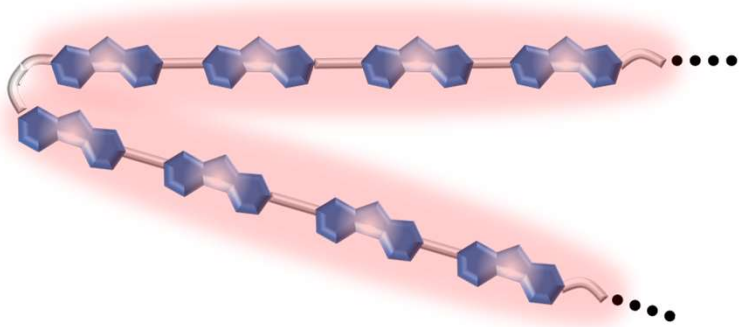


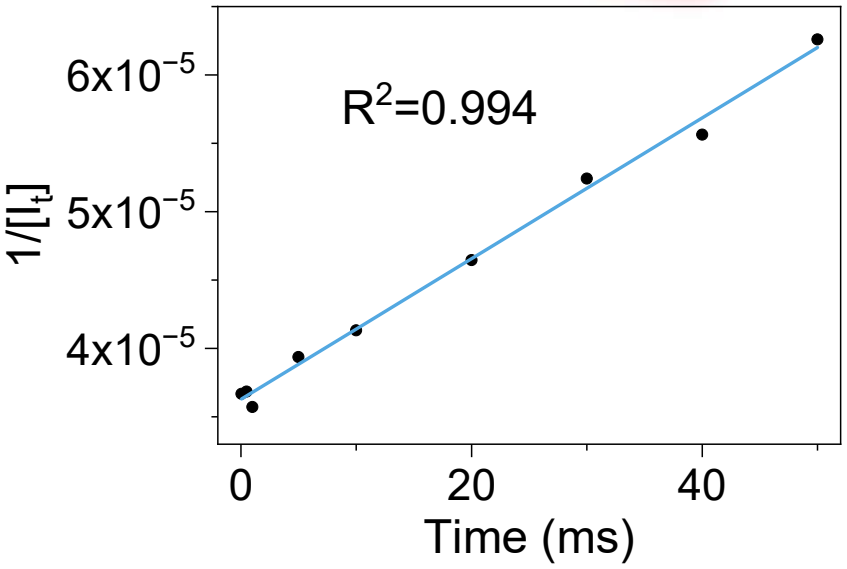




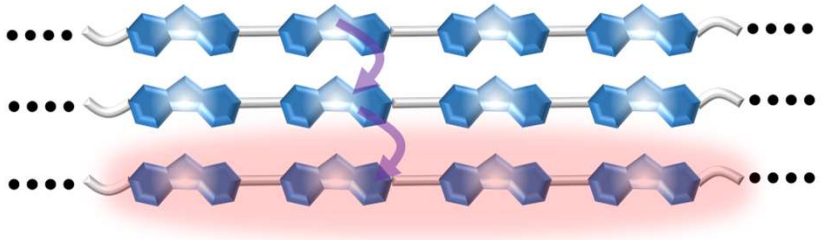
蓝光OLED容易变色的微观机制 (之一)

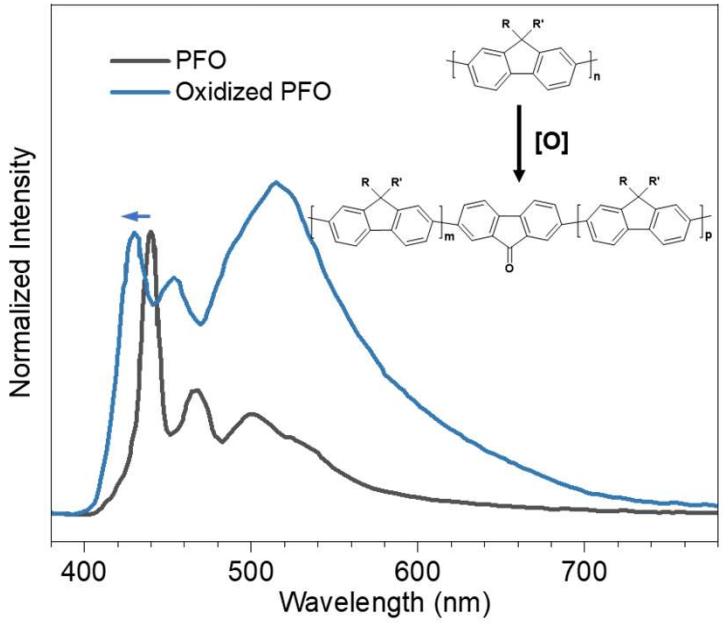
Triplet-Triplet Annihilation





Interchain Exciton Migration





轨道节点：波函数为零的位置也能成为设计参数

Orbital-Node Engineering

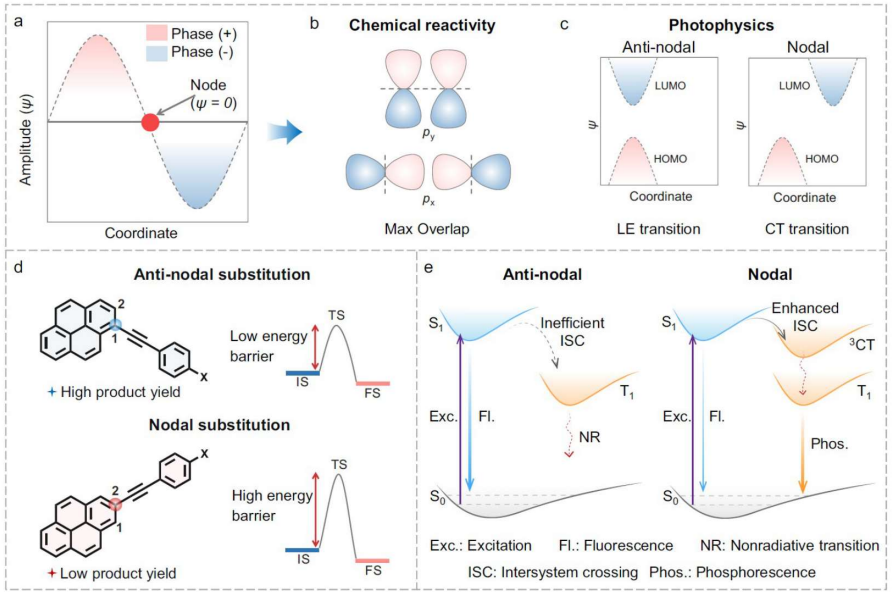
节点是轨道振幅为零的区域；它同时影响成键重叠、跃迁偶极与电荷离域。

1-位：反节点 / Antinode

轨道振幅大，共轭扩展与反应重叠更有利；荧光增强，但不利于 RTP。

2-位：节点 / Node

连接处电子解耦、几何扭曲，易形成 CT 态并增强 ISC，激活 RTP。



五年报告图 15 | 花的节点 / 反节点取代设计

来源：张国庆《2026 年最终报告》，2026 年轨道节点工作，图 15。

同一节点规则，连接宏观反应性与激发态自旋

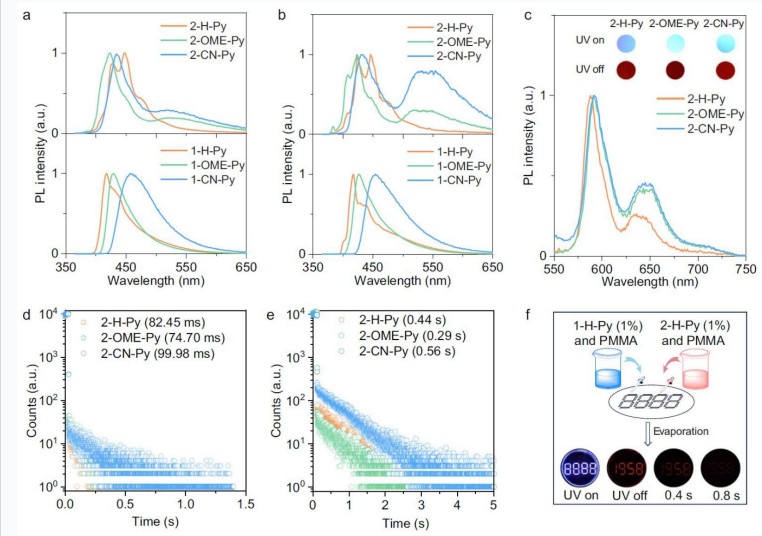
Connecting Reactivity and Excited-State Spin Dynamics

Sonogashira 偶联：反节点取代产率更高

体系	1-位	2-位
H-Py	76.8%	36.5%
OME-Py	85.4%	44.8%
CN-Py	62.8%	34.3%

氧化加成过渡态能垒：1-位 164 kJ/mol；2-位 193 kJ/mol。

节点取代：室温 RTP 寿命 80–100 ms，77 K 达 0.4–0.6 s；三重态可存续 >100 ns，而反节点异构体 <10 ns。



五年报告图 16 | 298/77 K 光谱、衰减与信息加密

来源：张国庆《2026 年最终报告》，G. Zhang et al., *Natl. Sci. Review* 2026年图 16 与节点效应数据。

矿物启发：把有机单分子锁进羟基磷灰石晶格

Mineral-Inspired Organic–Inorganic Hybrid Design

Ca^{2+}–羧酸根配位完成“离子锁定”，原位共沉淀 10 分钟内获得分子级分散的人工矿物。

31.1%

TPA-3COOH/HAP 的 RTP 量子产率

500 K

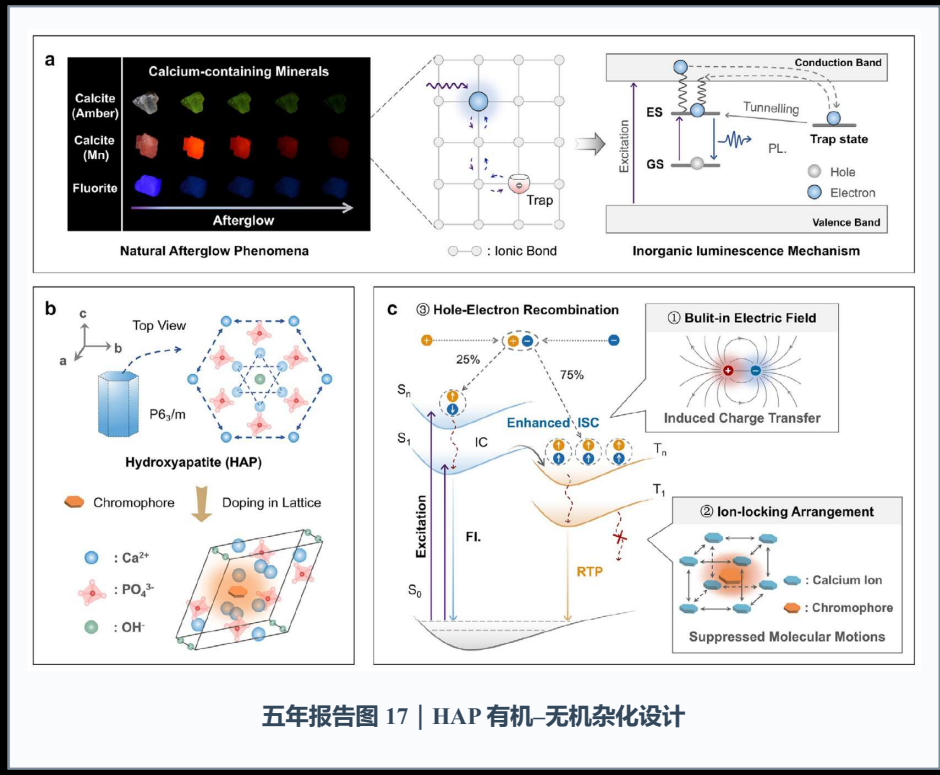
仍可观测有机磷光

303.7 ms

470 nm 磷光寿命

10 次循环

寿命仍保持在 370 ms 以上



五年报告图 17 | HAP 有机–无机杂化设计

来源：五年报告图 17–18；0.3 mol% TPA-3COOH/HAP。

内禀斯塔克电场：三重调控共同保护三重态

Intrinsic Stark Fields and Triplet Protection

① 电场诱导 CT

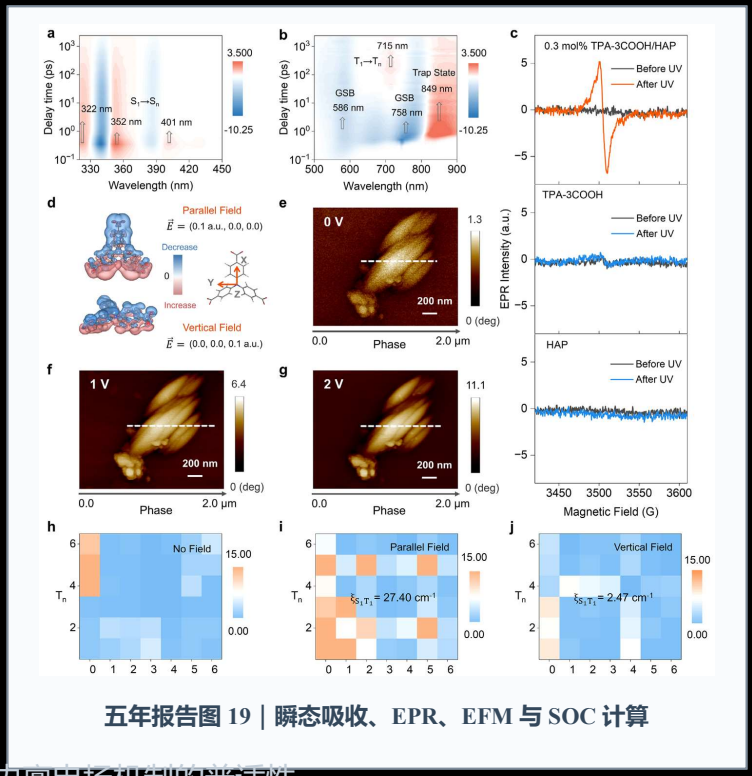
局域场约 10^{10}–10^{11} V/m；平行场使 ξS_1T_1 达 27.40 cm^{-1}，垂直场仅 2.47 cm^{-1}。

② 陷阱俘获—复合

浅陷阱约 0.125 eV；电荷复合按自旋统计可产生最高 75% 三重态。

③ 晶格限域保护

Ca^{2+} 离子锁与刚性晶格抑制非辐射失活；ISC 速率达 8.76×10^{10} s^{-1}。



五年报告图 19 | 瞬态吸收、EPR、EFM 与 SOC 计算

CaF_2、$CaCO_3$ 及多种羧基化发色团也可激活 RTP，支持局域内禀电场机制的普适性。

来源：张国庆《2026 年最终报告》，G. Zhang et al. Angew Chem 2026 图 19 与策略普适性。

04

近代物理进展 · 专题报告 / MODERN PHYSICS PROGRESS

最新进展：微相分离

LATEST PROGRESS: MICROPHASE SEPARATION

当能级相近仍无法解释发光差异时，还缺少哪一条设计规则？

建议讲授 / Time 11 分钟 + 讨论

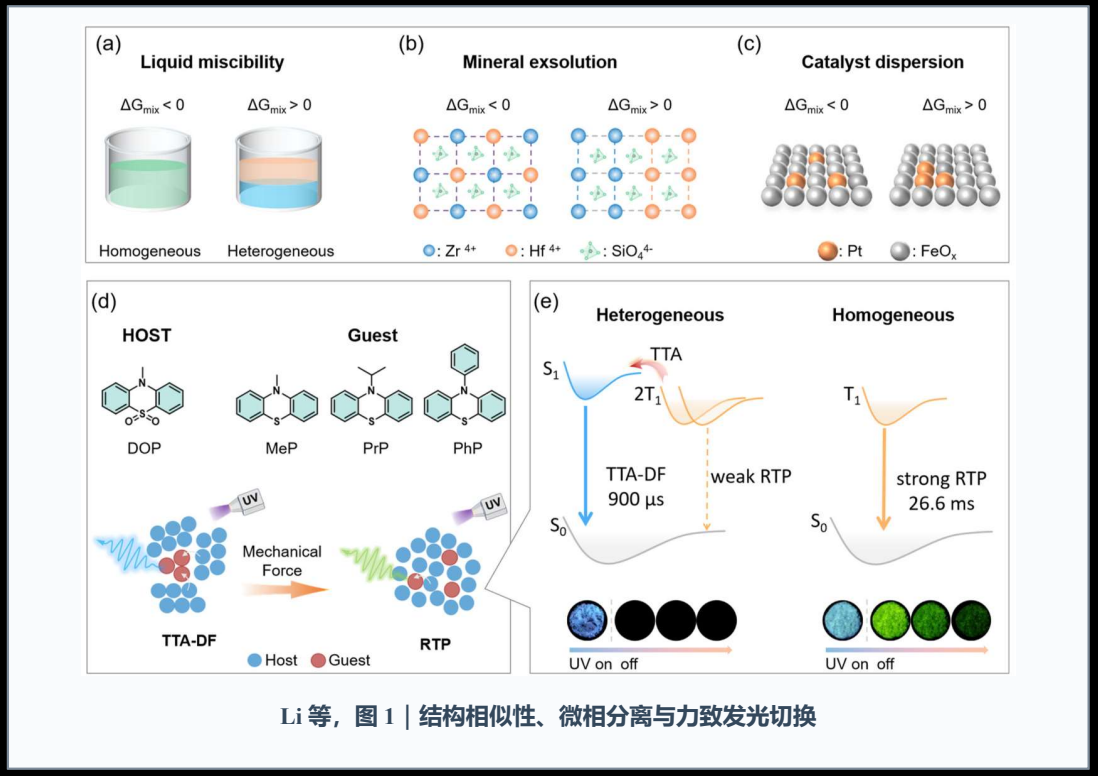
最新论文：把“相似相溶”引入有机 RTP 设计

Structural Similarity and Microphase Separation

主客体能级匹配已经足够，为什么不同掺杂晶体的 RTP 仍相差巨大?

- 主体：吩噻嗪二氧化物 DOP。
- 客体：MeP、PrP、PhP，N-取代基逐步增大。
- 变量：结构相似性与混合自由能 ΔGmix。

相似 → 分子级固溶体 → RTP
不相似 → 微相分离 → TTA-DF



Li 等，图 1 | 结构相似性、微相分离与力致发光切换

来源：Li et al., Angew. Chem. Int. Ed. 2026, 65, e4780761，图 1；DOI: 10.1002/anie.4780761。

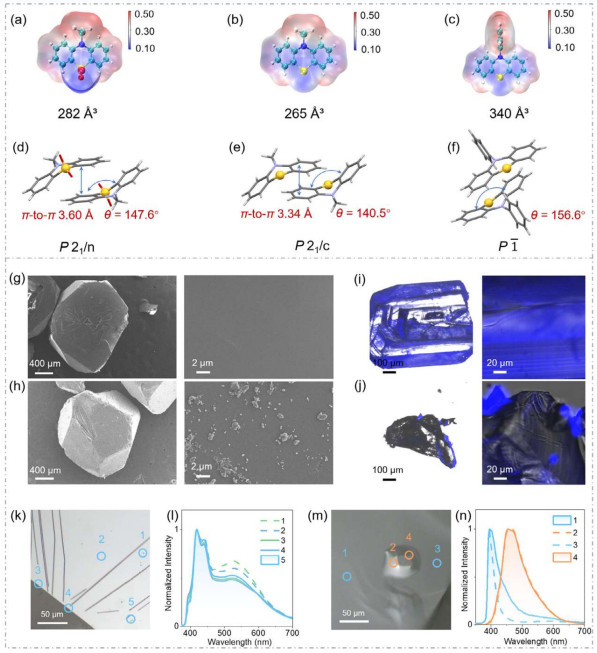
能级相近不等于固体相容：显微证据确认微相分离

Morphological Evidence for Like Dissolves Like

DOP 的 T_1 为 2.72 eV；三种客体的 T_1 为 1.99–2.05 eV，均满足主体到客体的 TTET。

- MeP/DOP：表面均匀，微区光谱基本一致。
- PhP/DOP：出现颗粒微区，CLSM 呈亮斑 / 暗背景。
- 结构失配驱动热力学微相分离，而非能级失配。

关键新增变量：主客体相容性控制激子的空间浓度。



Li 等，图 3 | 晶体结构、SEM、CLSM 与微区光谱

来源：Li et al., Angew. Chem. Int. Ed. 2026, 65, e4780761，图 2–3。

微相分离切换 RTP 与 TTA-DF；研磨可部分逆转

Phase Separation Switches RTP and TTA Delayed Fluorescence

34.5%

MeP/DOP：结构相似，RTP 量子产率

0.4%

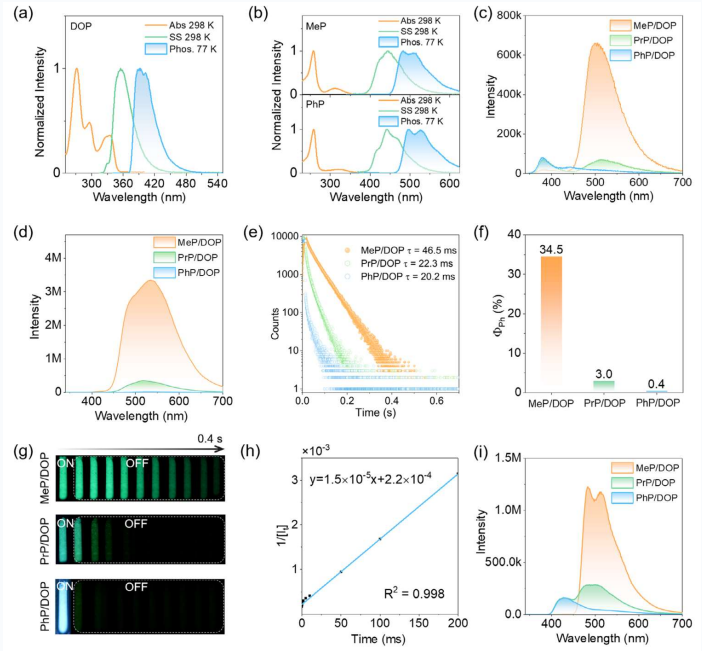
PhP/DOP：结构不相似，RTP 量子产率

同主体、同掺杂量下，RTP 量子产率相差近 87 倍

MeP/DOP：535 nm，46.5 ms

PhP/DOP：539 nm，20.2 ms

温和研磨使 PhP/DOP 部分无定形化，RTP 强度提高约 24 倍



Li 等，图 4 | 掺杂晶体的光谱、衰减与量子产率

来源：Li et al., Angew. Chem. Int. Ed. 2026, 65, e4780761，图 4–5；1 mol% 掺杂，298 K。


有机分子光电磁实验室 (Est. since 2011)

谢谢 · 讨论

Thank You · Discussion

能否把分子结构、局域电场、聚集尺寸与手性，
写成同一套可预测的激发态动力学？

轨道 · 电场 · 自旋 · 聚集 · 热力学

Orbitals · Fields · Spin · Aggregation

报告主线 / Narrative

1. 新物种：光致基态电荷转移复合物
2. 新基准：ppb 杂质与非结晶溶剂标准
3. 新动力学：手性、冰相、轨道与电场
4. 新规则：聚集尺寸与结构相似性
5. 前沿：电荷转移与手性自旋选择

内容来源：五年报告、2026 版申请书

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