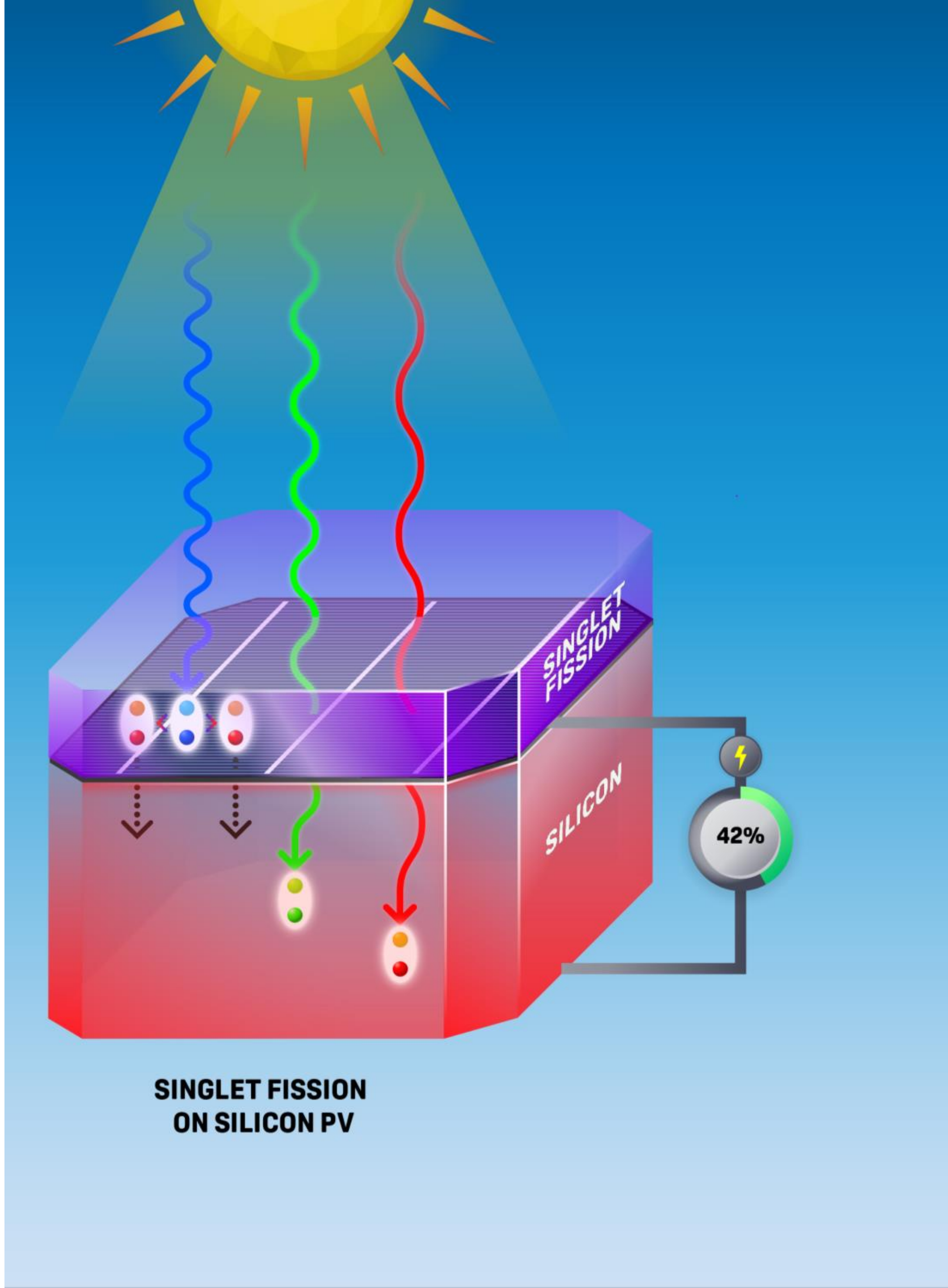
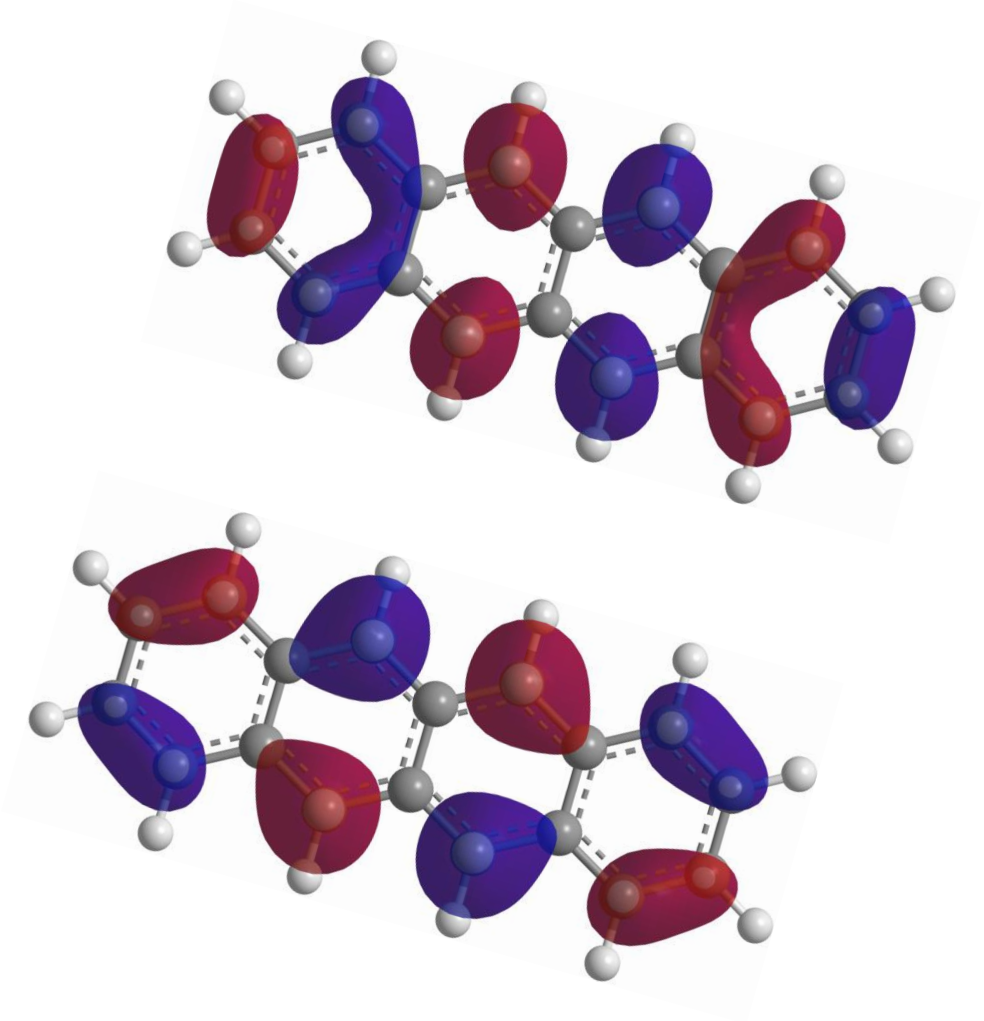
OMEGA Silicon: Toward a singlet fission silicon tandem solar cell

Dr Murad Tayebjee
https://www.omegasilicon.solar/

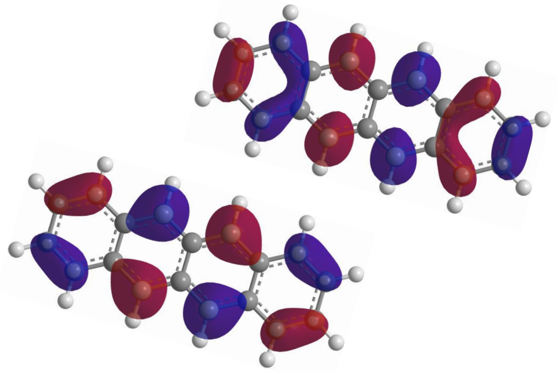


Outline

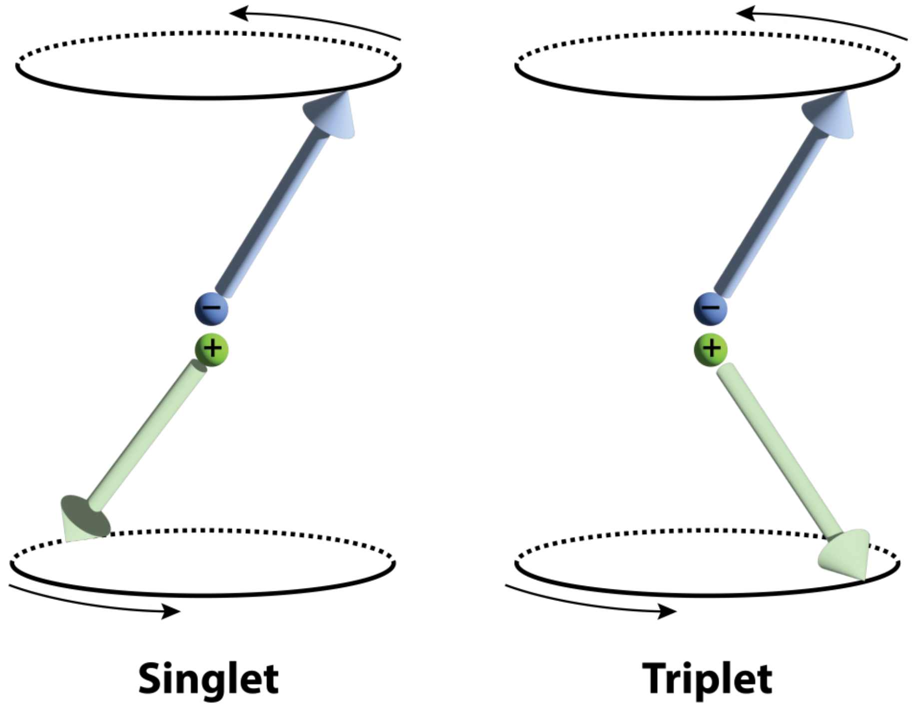
- ❑ Molecular semiconductors: a crash course



Outline

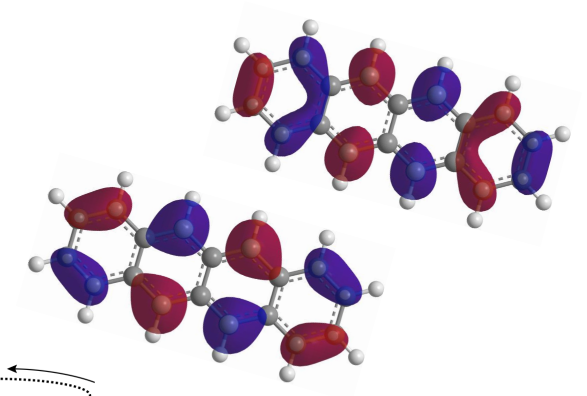


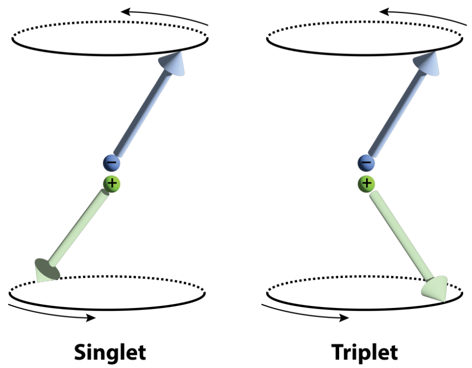
- ❑ Molecular semiconductors: a crash course
- ❑ Singlets & triplets

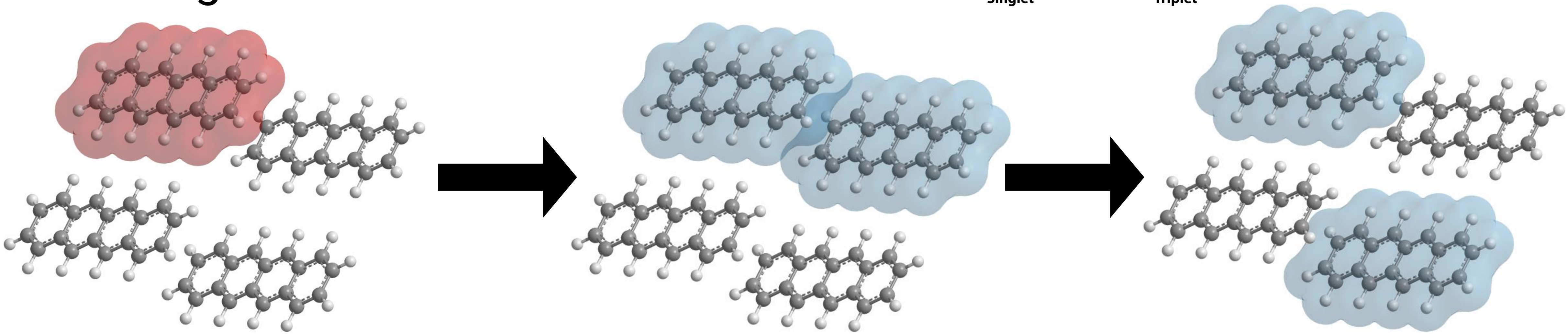


Outline

- ❑ Molecular semiconductors: a crash course
- ❑ Singlets & triplets
- ❑ Singlet fission

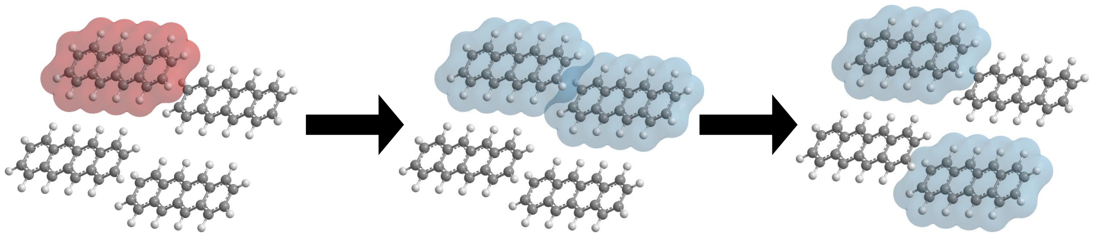


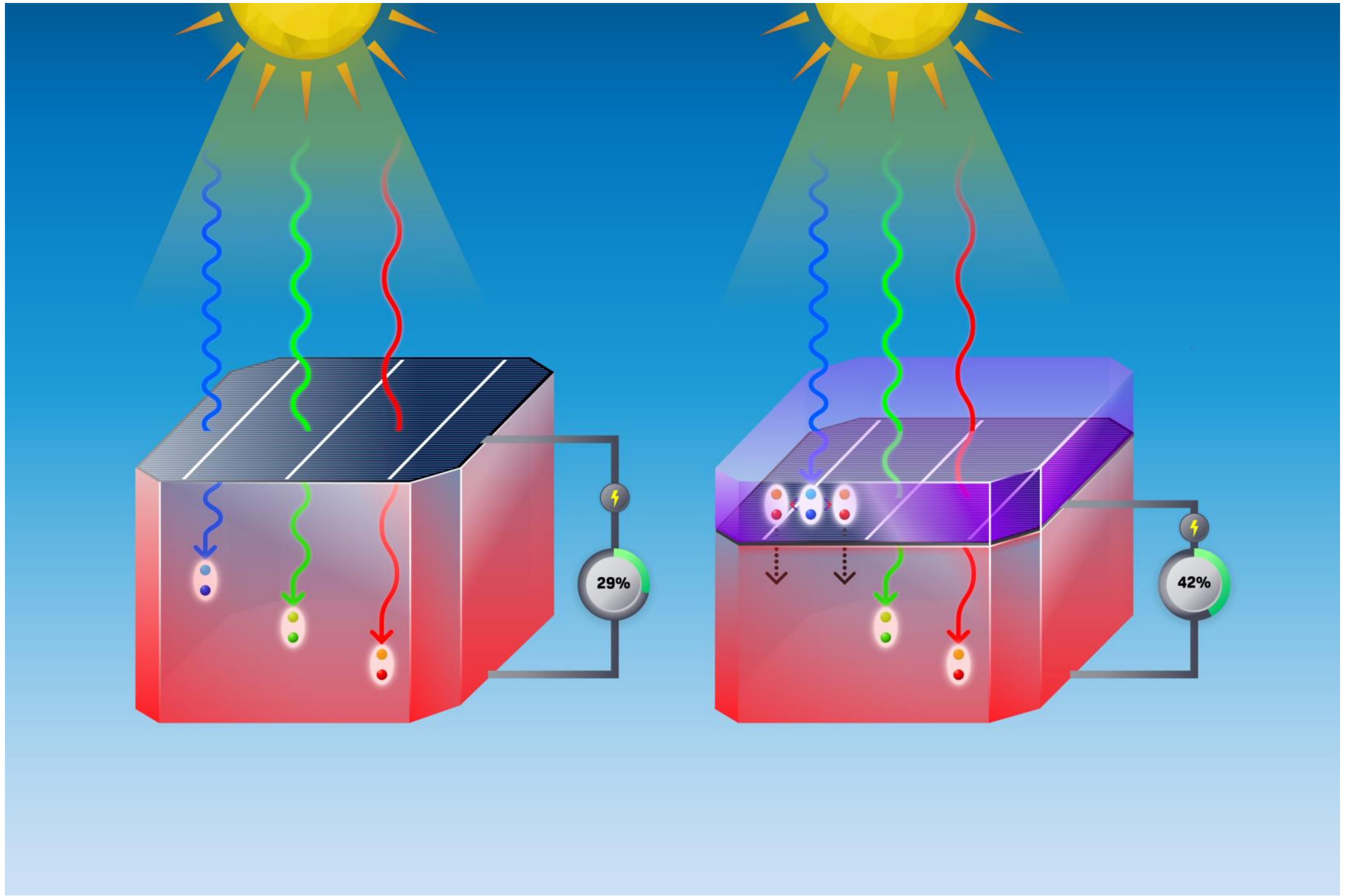




Outline

- ❑ Molecular semiconductors: a crash course
- ❑ Singlets, triplets, and spin
- ❑ Singlet fission
- ❑ Singlet fission for photovoltaics

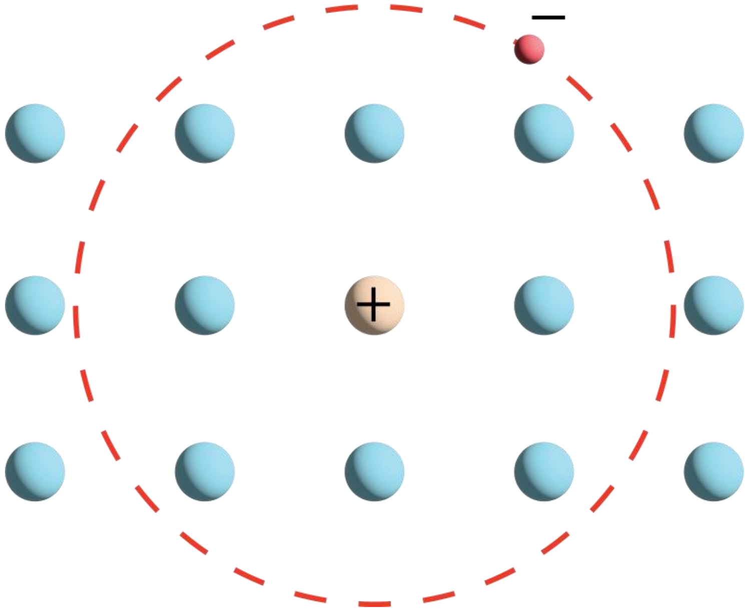




Comparing Semiconductors

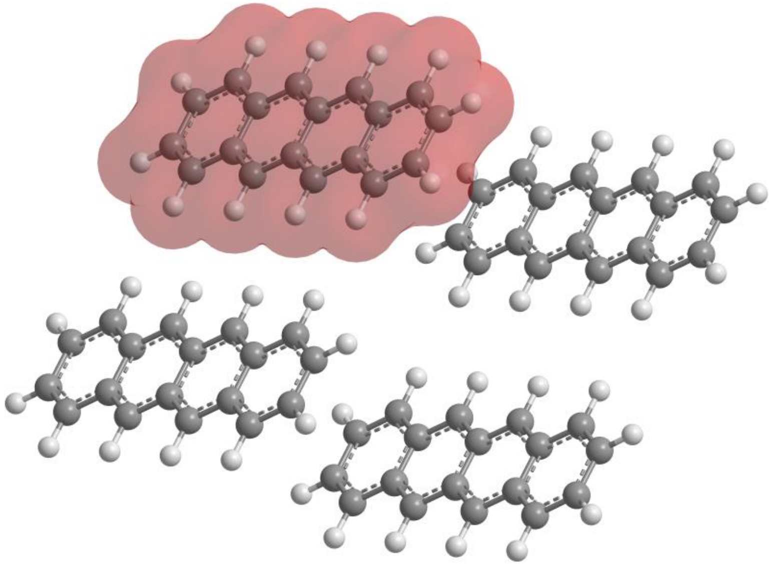
Inorganic

- Wannier Excitons



Organic

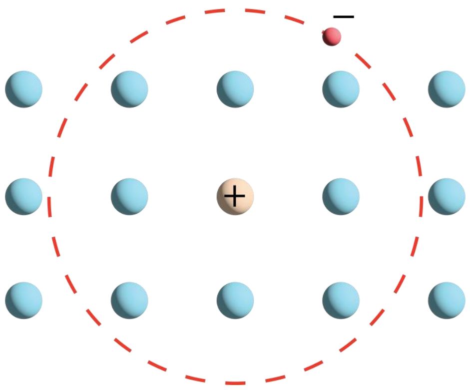
- Frenkel Excitons



Comparing Semiconductors

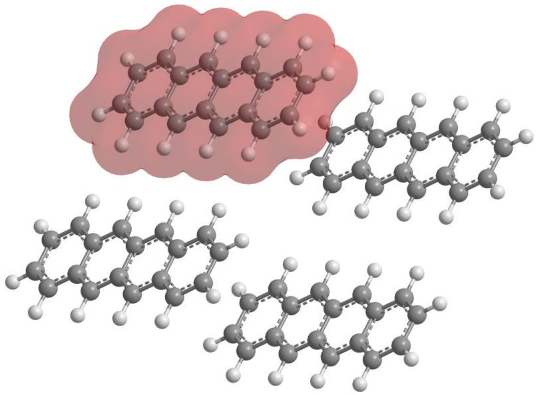
Inorganic

- Wannier excitons
  - Weakly bound (~0.1eV)
  - Higher dielectric constant
  - Better charge mobility

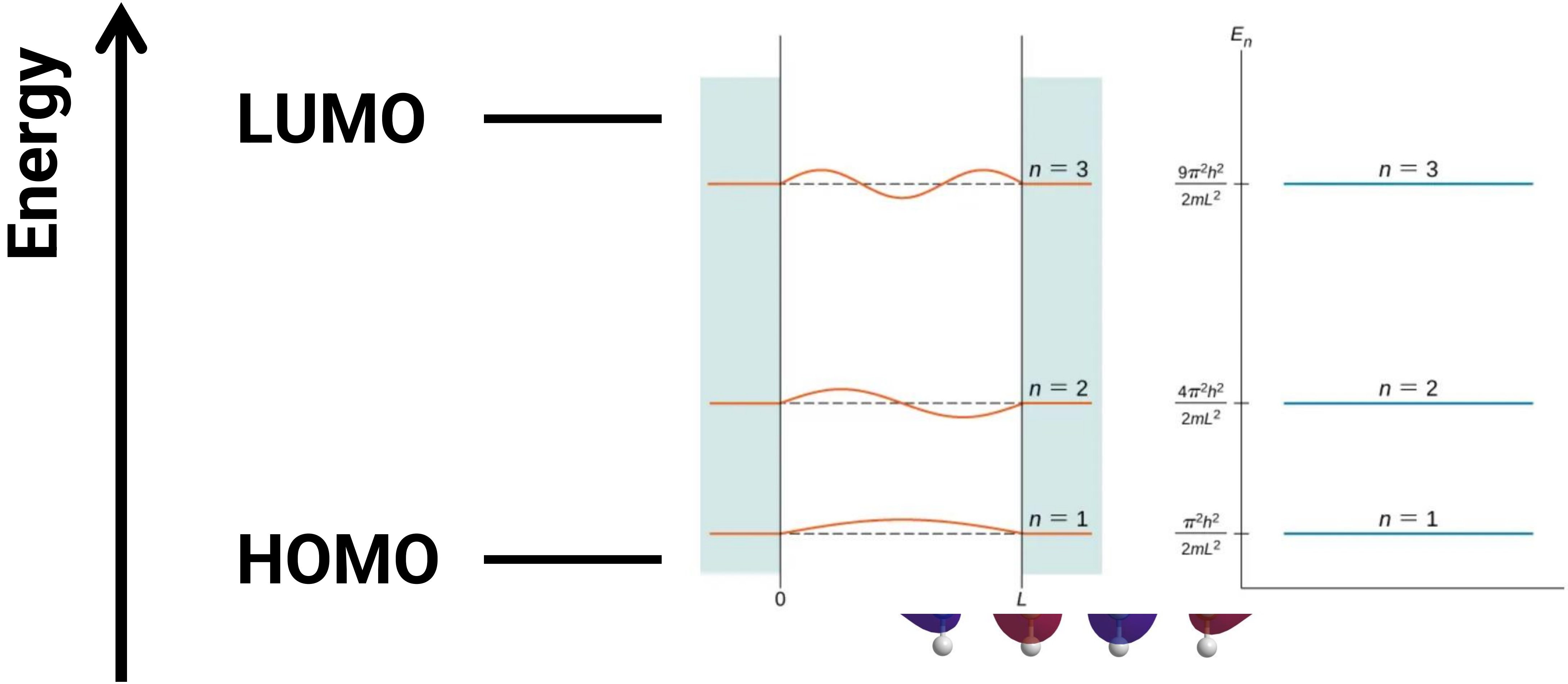


Organic

- Frenkel Excitons
  - Strongly bound (~1eV)
  - Lower dielectric constant
  - Worse charge mobility

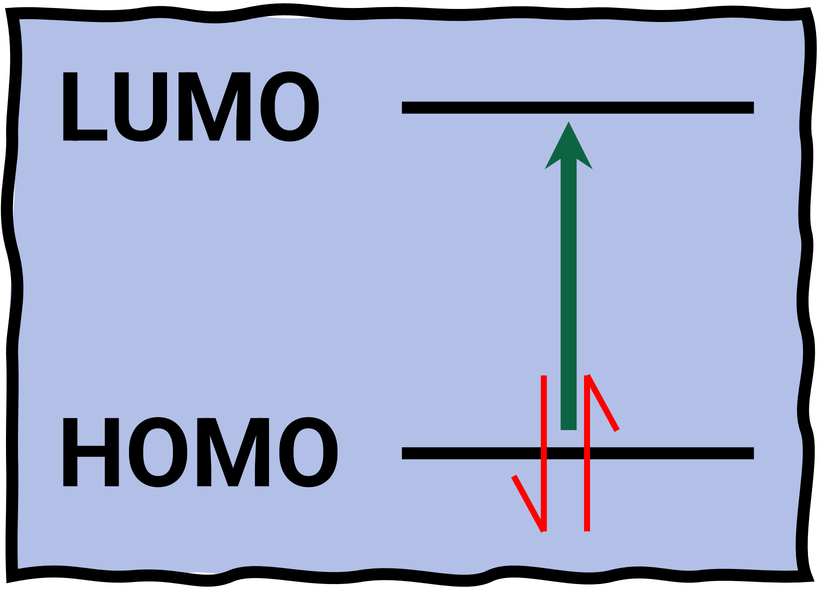


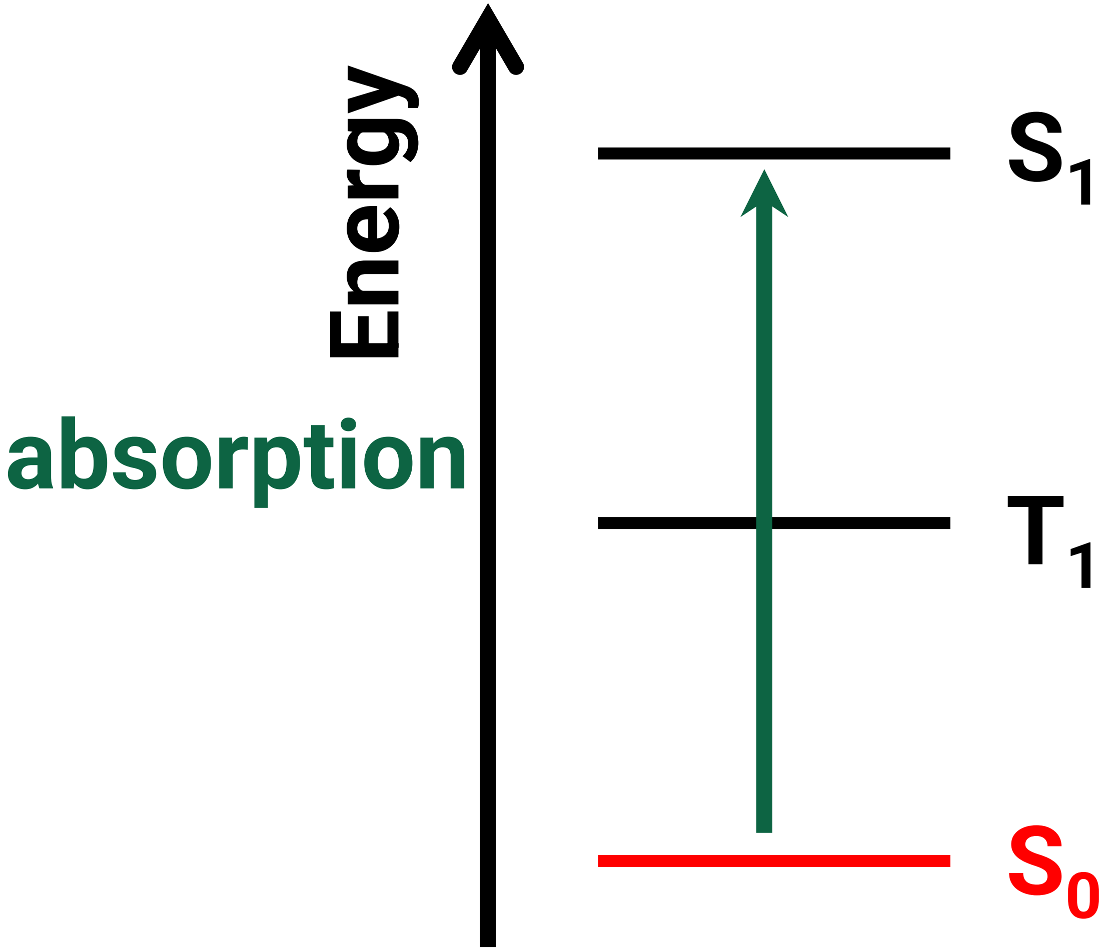
Molecular orbitals



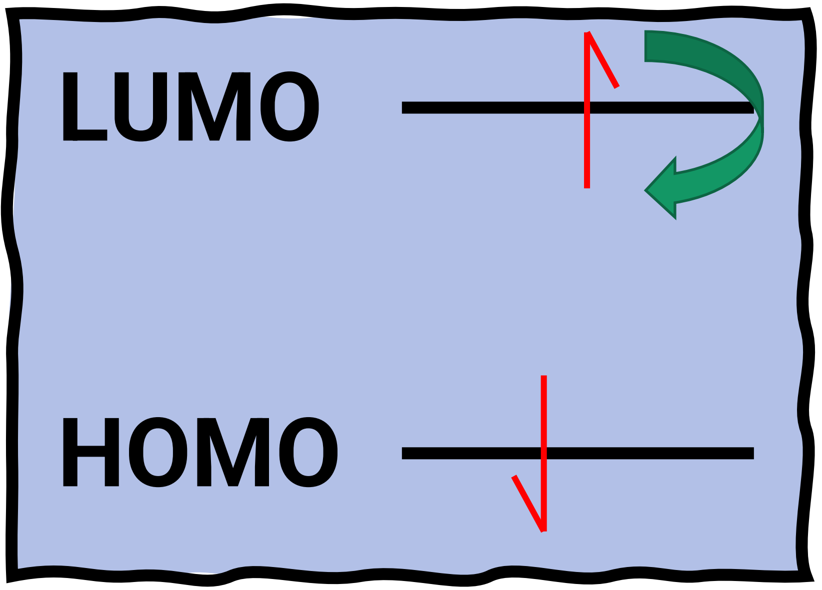
https://openstax.org/books/university-physics-volume-3/pages/7-4-the-quantum-particle-in-a-box

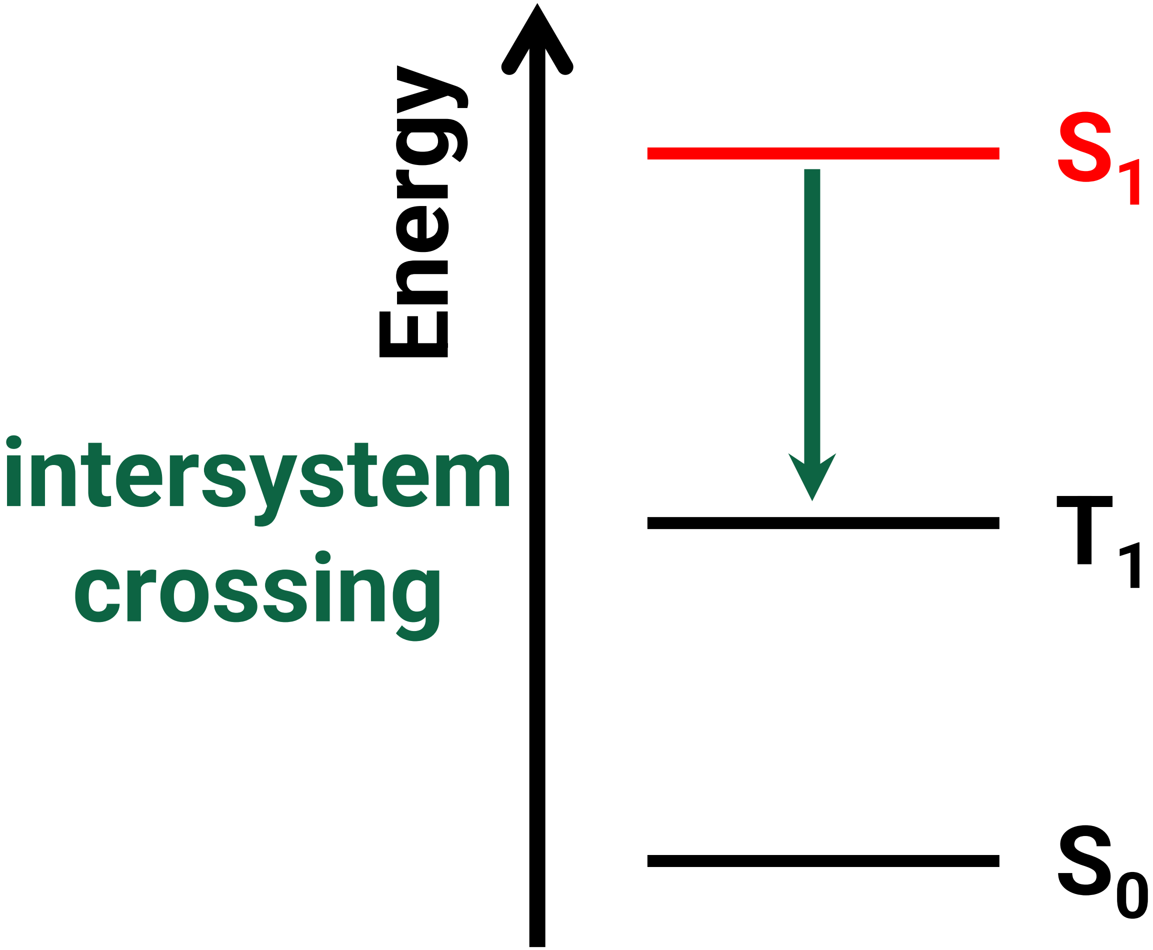
Molecular states



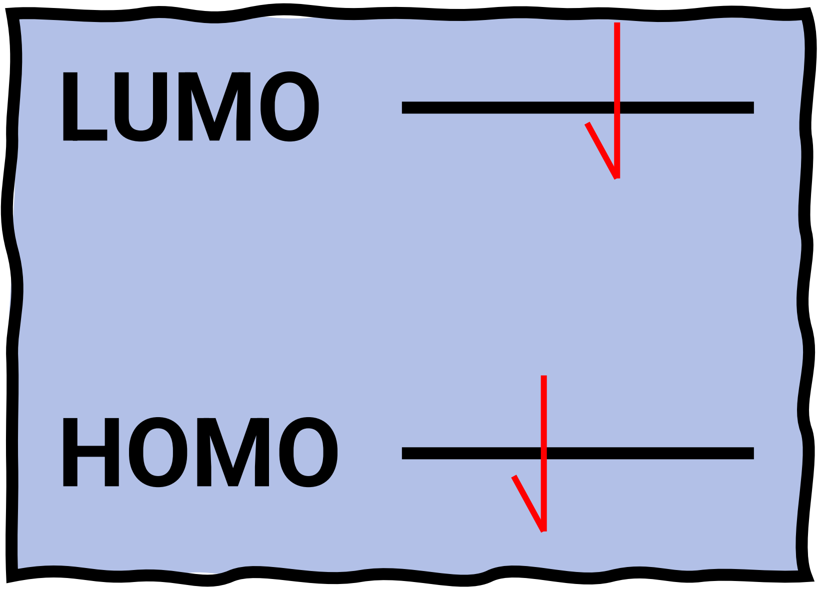


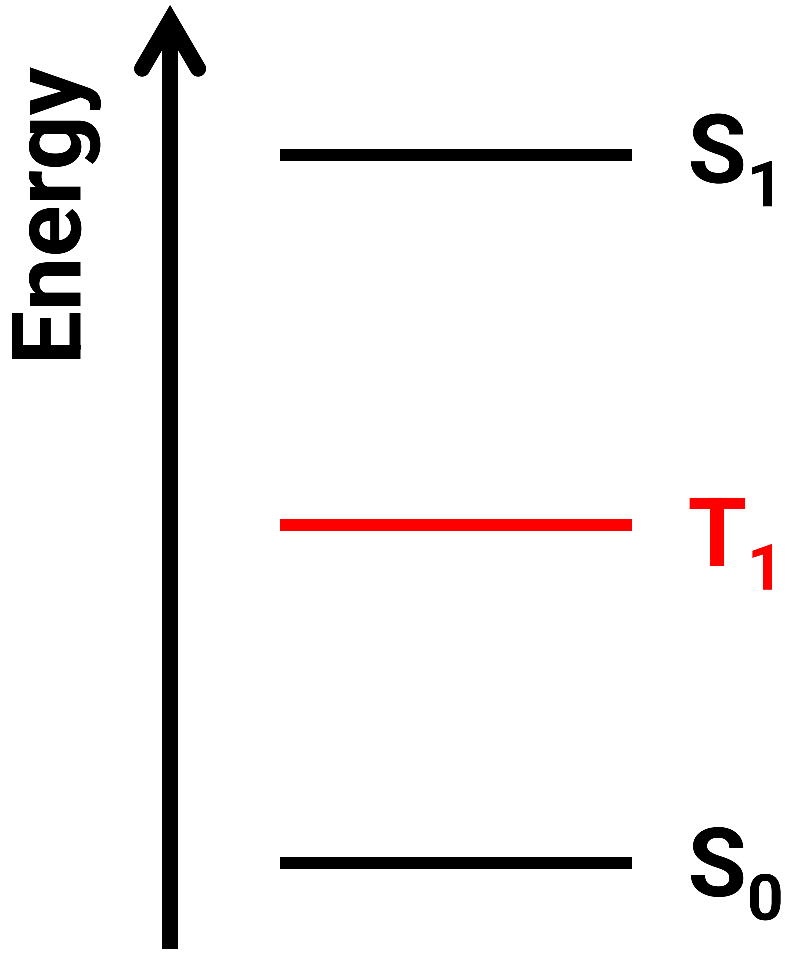
Molecular states



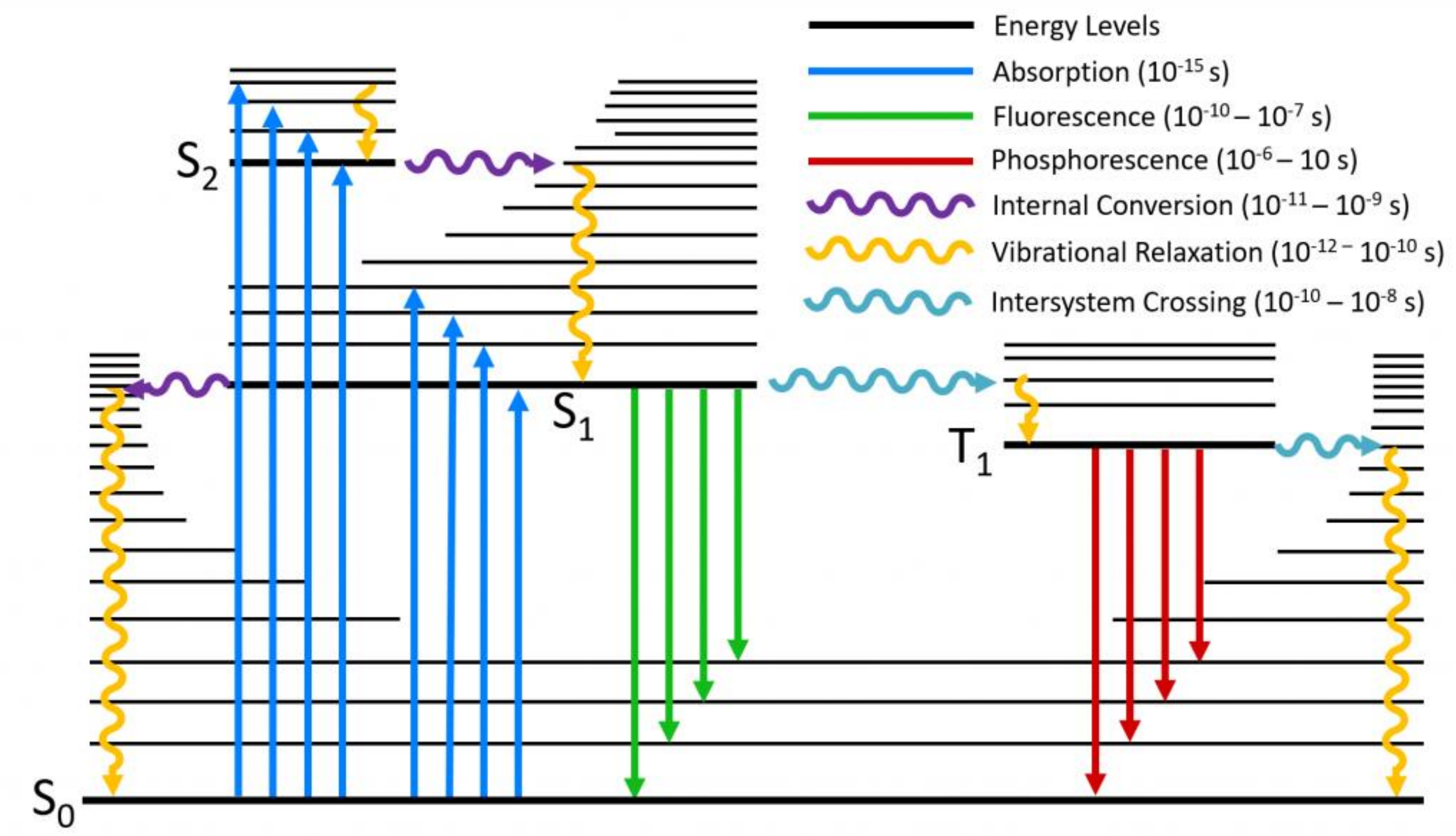


Molecular states



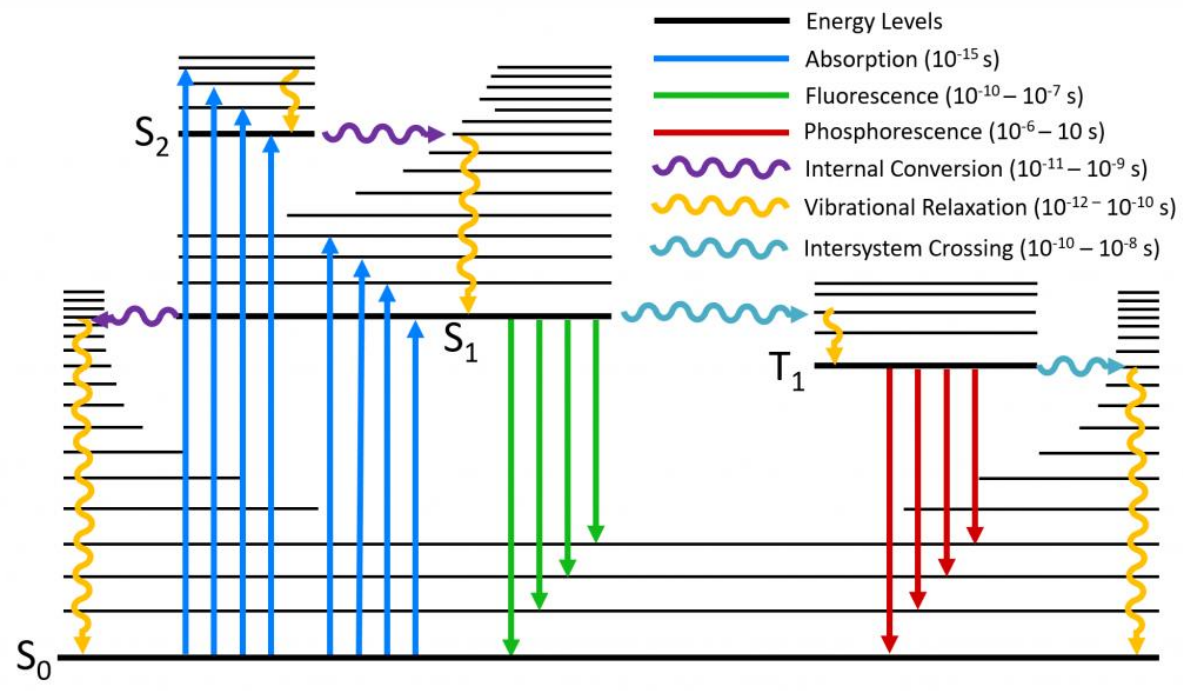


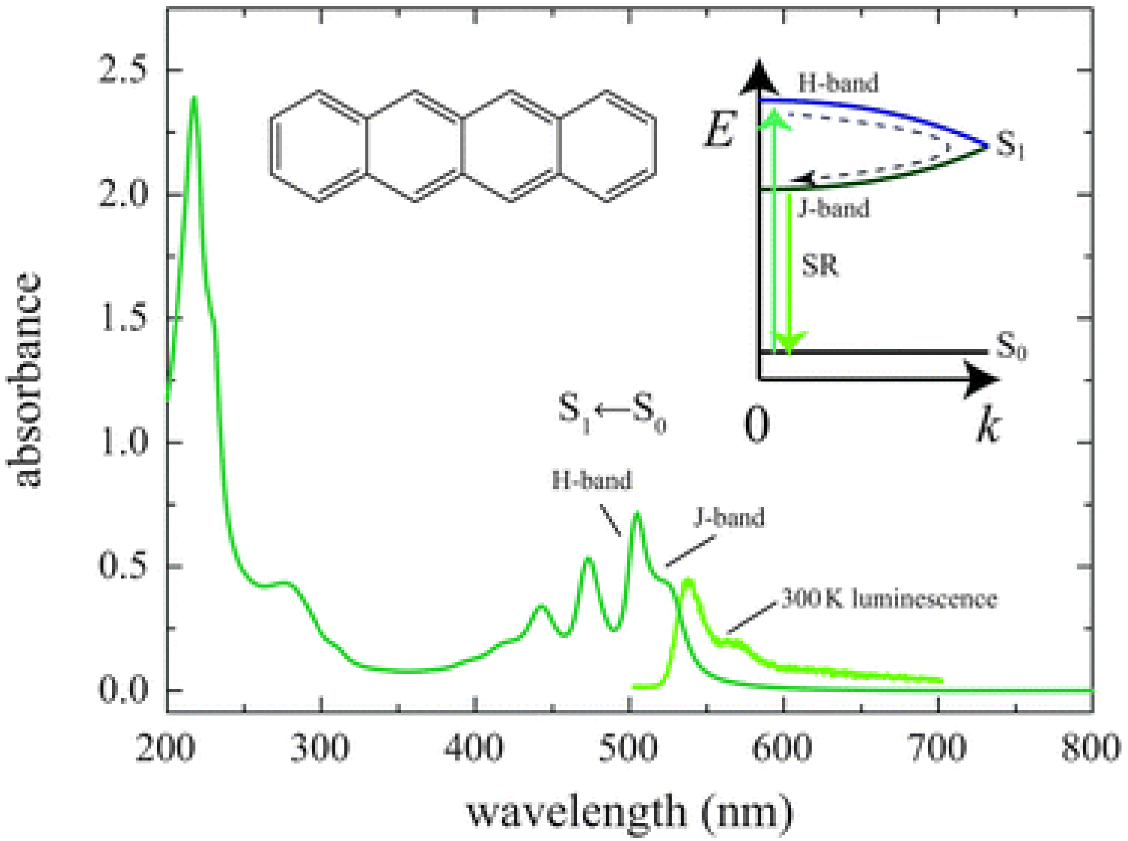
The Jablonski Diagram



https://www.edinst.com/blog/jablonski-diagram-2/

The Jablonski Diagram



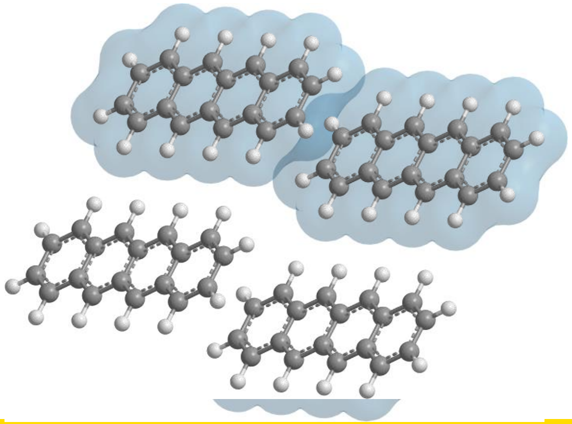


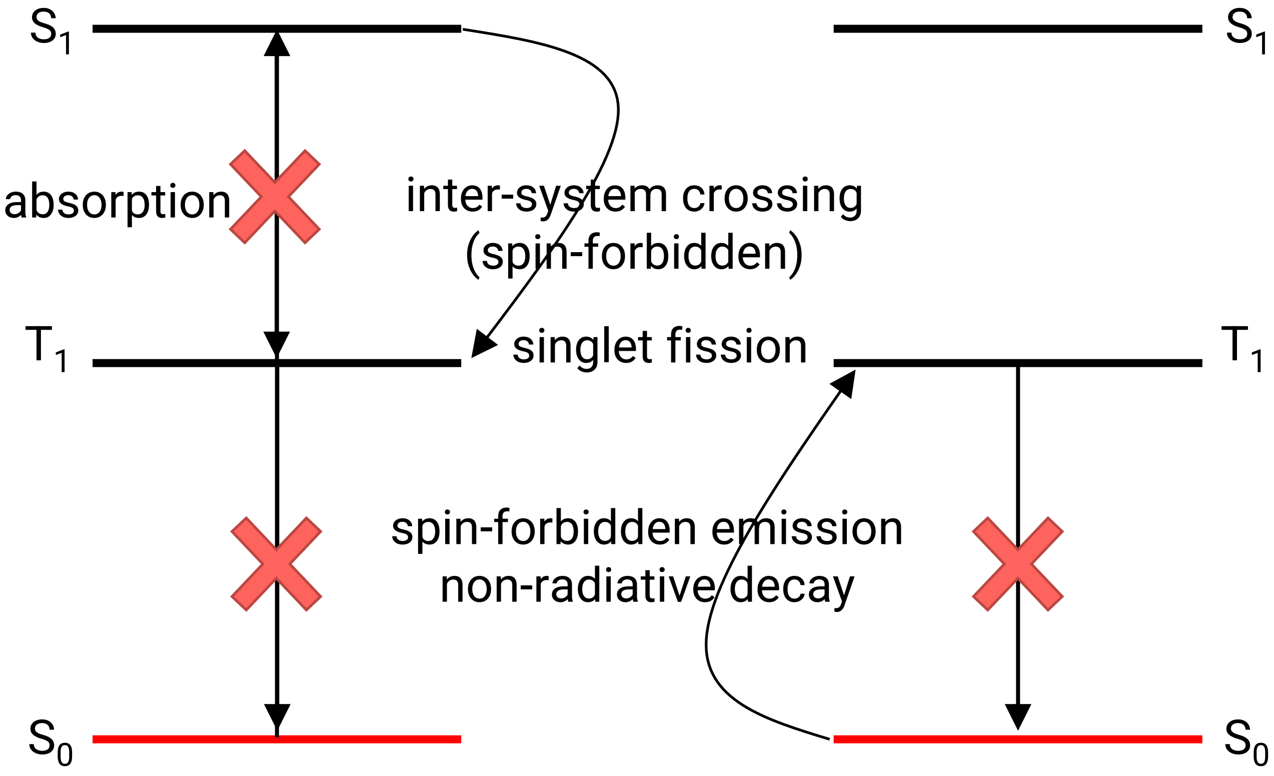
Tayebjee, M. J. Y.; Clady, R. G. C. R.; Schmidt, T. W. *Physical Chemistry Chemical Physics* **2013**, *15* (35), 14797.

https://www.edinst.com/blog/jablonski-diagram-2/

Singlet Fission – Organic Multiple Exciton Generation

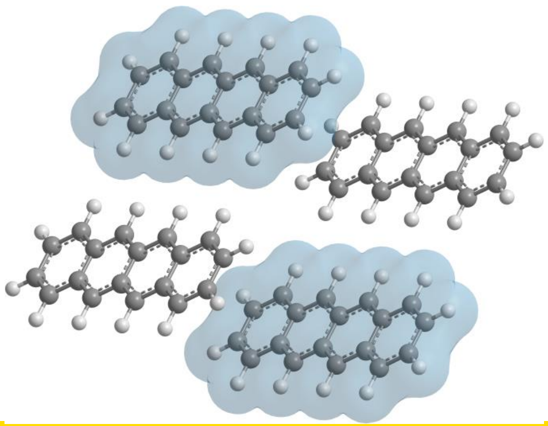
- Fast (fs-ps)
- 200% yield of long-lived triplet excitons**
- **One** photon yields **two** electron-hole pairs!

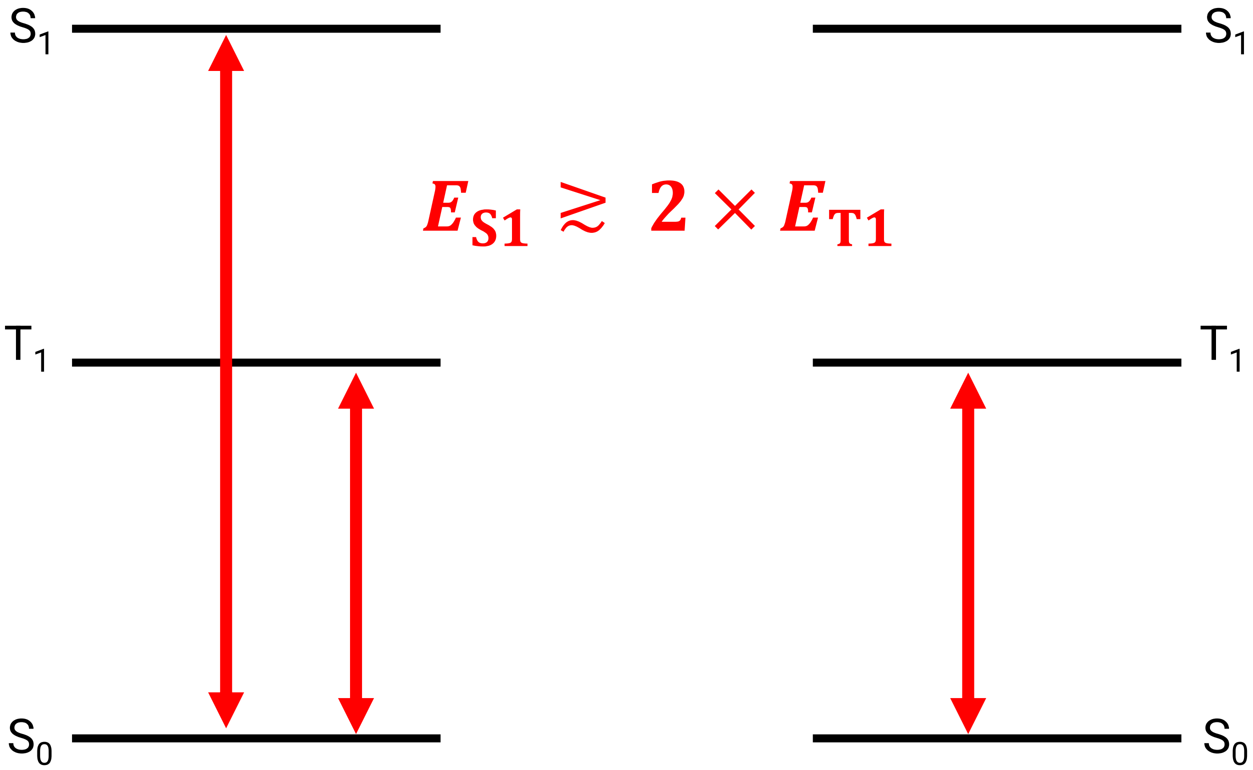




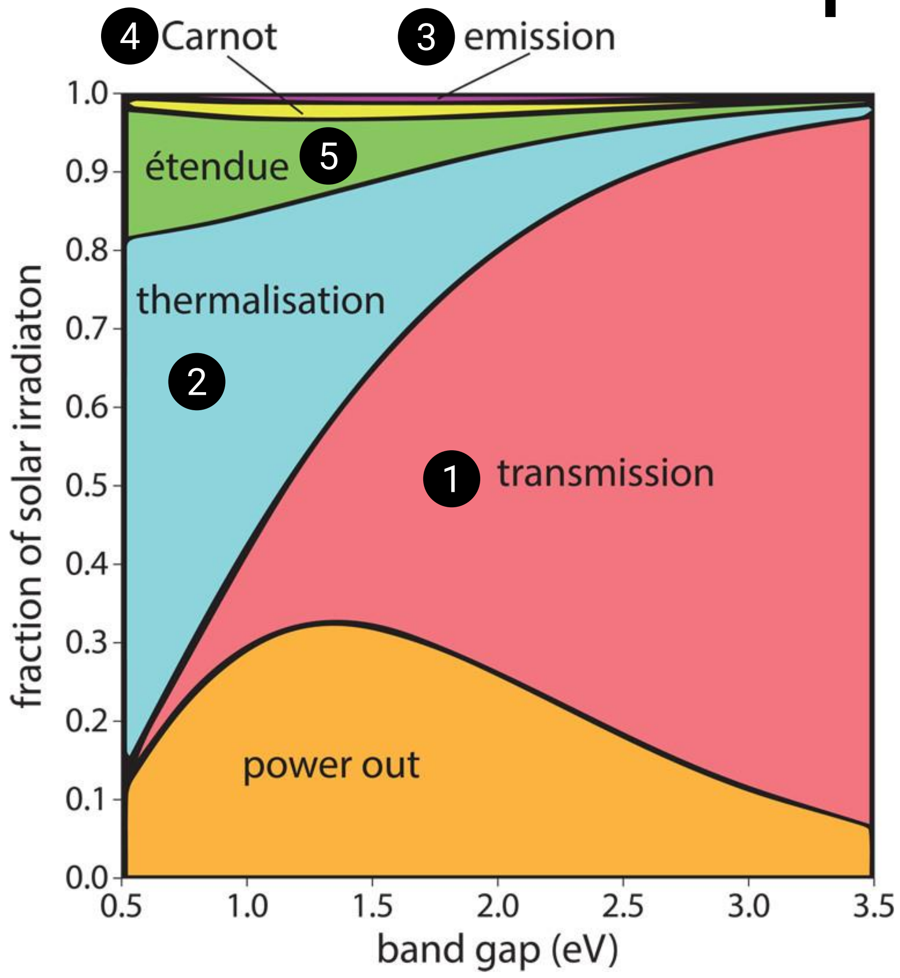
Singlet Fission – Organic Multiple Exciton Generation

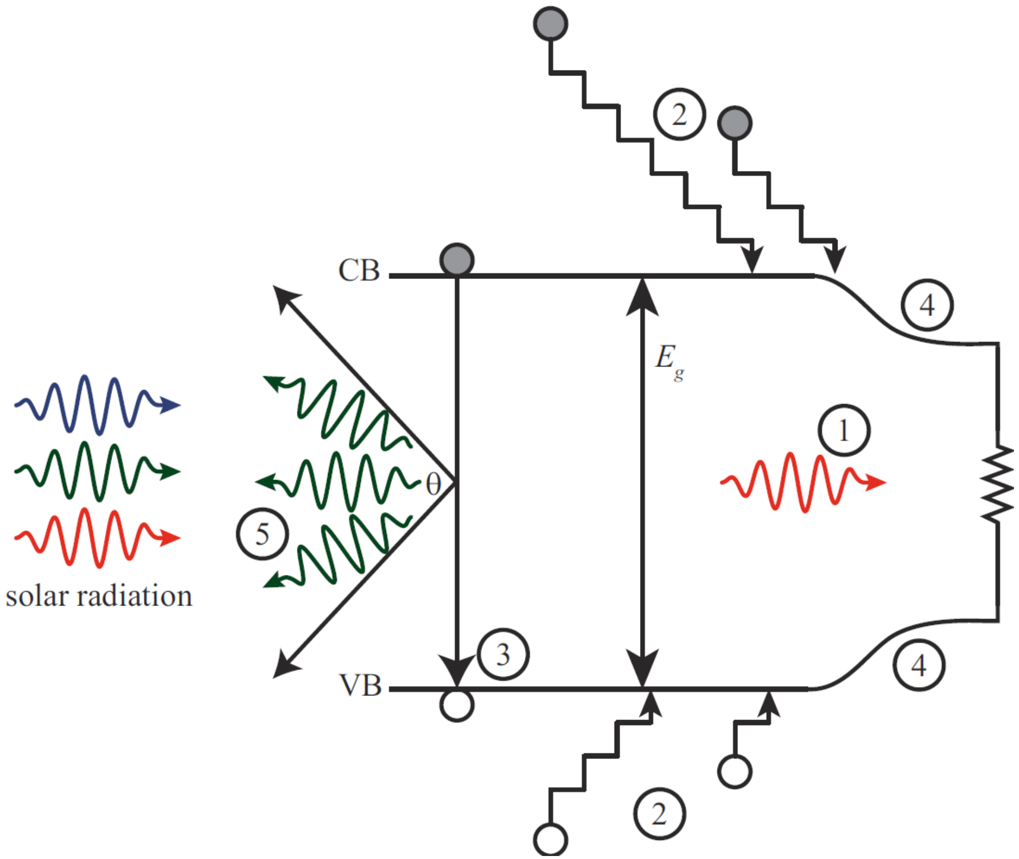
- Fast (fs-ps)
- 200% yield of long-lived triplet excitons**
- **One** photon yields **two** electron-hole pairs!





How will this help PV?

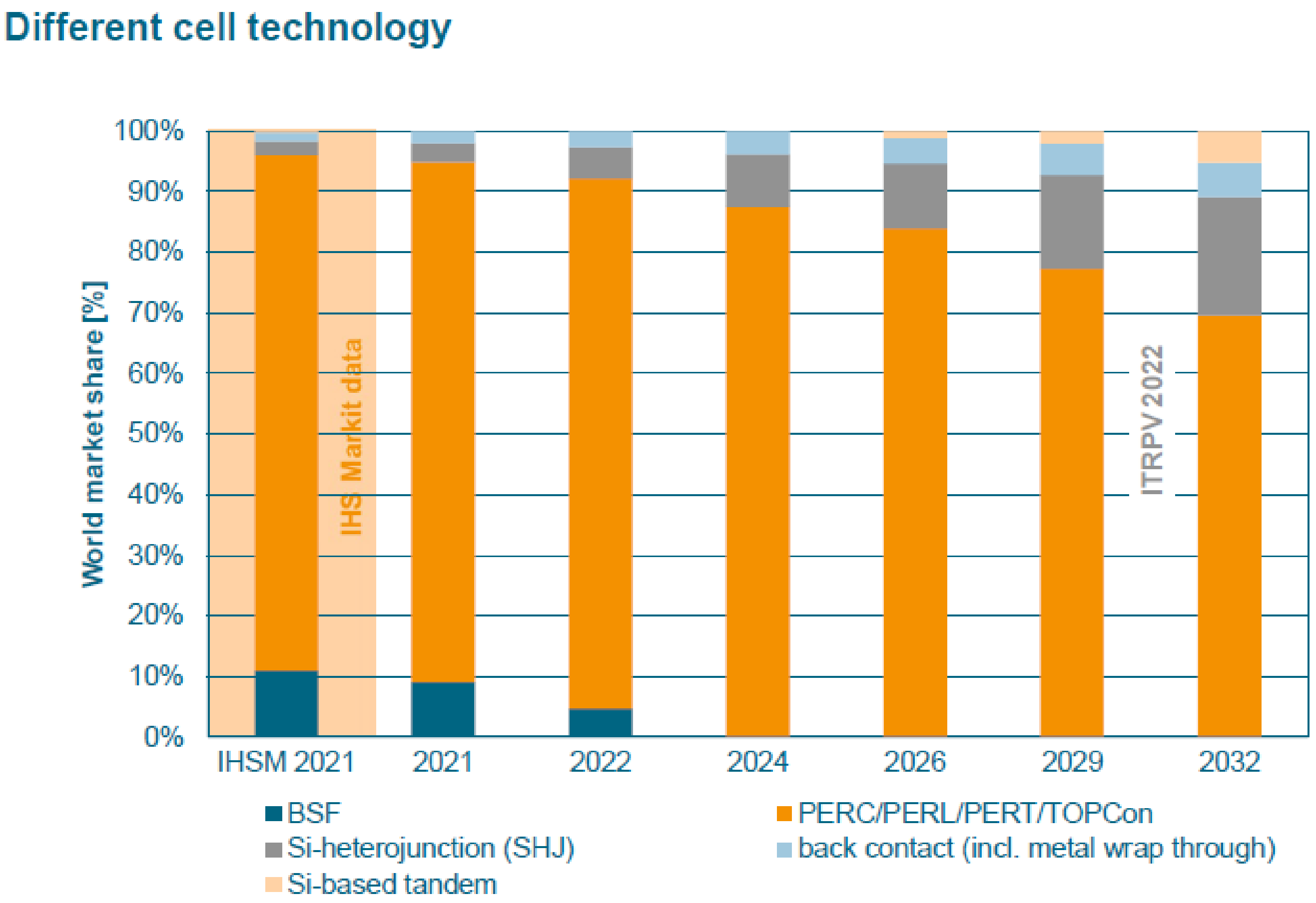




Adapted from: Green, M. A. *Progress in Photovoltaics: Research and Applications* **2001**, *9* (2), 123–135.

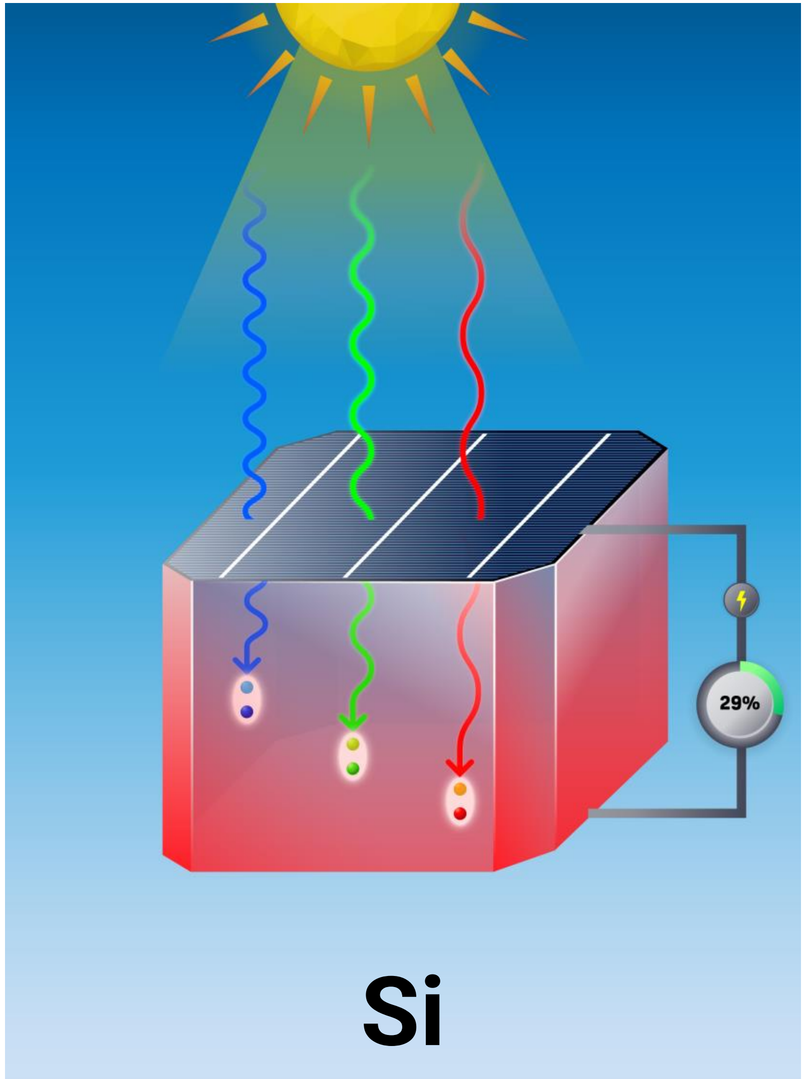
Hirst, L. C.; Ekins-Daukes, N. J. *Progress in Photovoltaics: Research and Applications* **2011**, *19* (3), 286–293.

Something-on-silicon



Ω SILICON

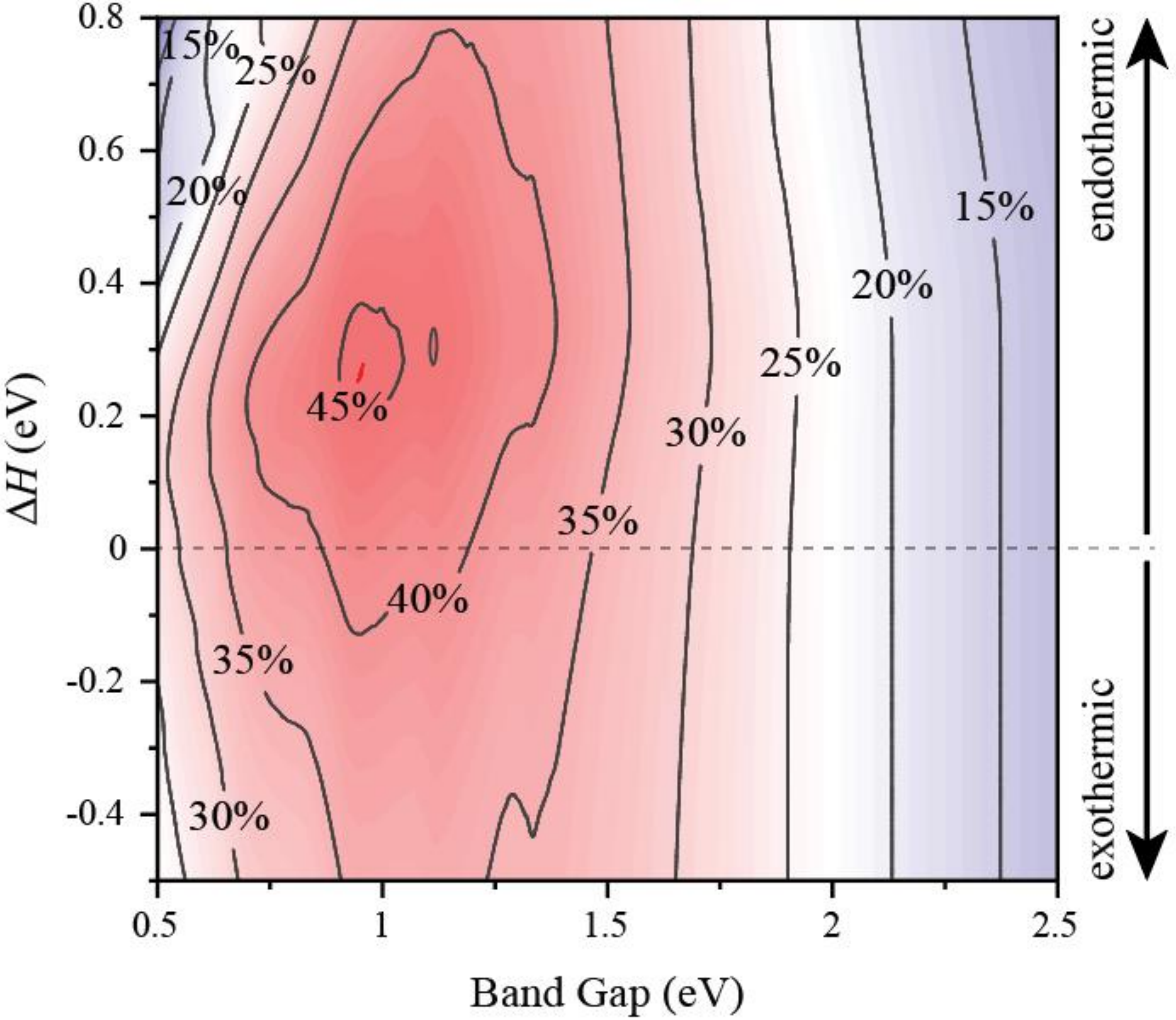
- **O**rganic
- **M**ultiple
- **E**xciton
- **G**eneration
- **A**ugmented
- **Si**licon



UNSW SYDNEY

Ω SILICON

- **O**rganic
- **M**ultiple
- **E**xciton
- **G**eneration
- **A**ugmented
- **S**ilicon



Tayebjee, M. J. Y.; Gray-Weale, A. A.; Schmidt, T. W.. *J Phys Chem Lett* **2012**, *3* (19), 2749–2754.

Prof. Ned Ekins-Daukes

PROJECT LEAD

Prof. Timothy Schmidt

SCIENTIFIC DIRECTOR

Dr Murad Tayebjee

DEPUTY PROJECT LEAD

Prof. Dane McCamey

CHAIR - PROJECT BOARD

Dr Jessica Yajie Jiang

INDUSTRIAL LIAISON and OPTICAL INTEGRATION LEAD

Prof. Bram Hoex

INTERFACE LEAD

Dr Alison Ciesla

MODULE INTEGRATION, TESTING AND RELIABILITY LEAD

Dr Michael Nielsen

DEVICE INTEGRATION LEAD

Dr Phoebe Pearce

MODELLING LEAD

A/Prof. Jon Beves

ORGANIC SYNTHESIS LEAD

Dr Nathan Chang

TECHNO-ECONOMIC ANALYSIS LEAD

Dr Young Cho

Project Manager

Alexander Baldacchino, Matthew Brett, Jingnan (Taffy) Tong, Shona McNab, Ben Carwithen, Alvin Mo

8 Industry Partners

DASOLAR 一道新能

JINERGY

JinKO Solar

JA SOLAR

阿特斯

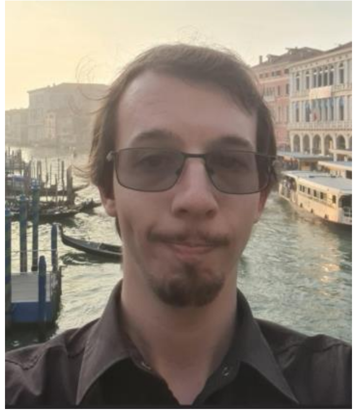
中来股份 JOLYWOOD

Xinhao Energy

Leadmicro 微导

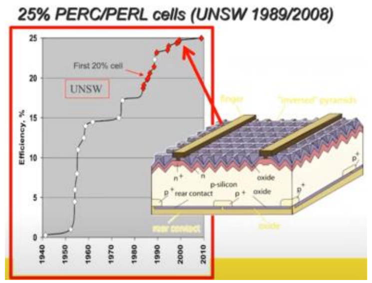
Advantages of ΩSi

- No electric transport in top "cell"
- Can use existing silicon devices, an add only an additional top later
- No need to current/voltage match
- Minimal changes to the silicon PV architecture
- Radiative device can even use the same passivation as existing Si technologies
- Materials will likely be scalable using existing OLED synthesis techniques



Baldacchino, A. J.; Collins, M. I.; Nielsen, M. P.; Schmidt, T. W.; McCamey, D. R.; Tayebjee, M. J. Y. *Chemical Physics Reviews* **2022**, *3* (2), 21304.
https://www.pv-magazine-australia.com/2022/04/28/unsw-exclusive-unlocking-the-potential-of-singlet-fission-for-future-pv-devices/

So why isn't ΩSi Prevalent?



1953 – Silicon solar cell demonstrated

1974 – Martin Green starts PV research at UNSW

$100/$W_p$ 10%

1983 – PERC solar cell invented

$10/$W_p$ 15%

1989 – PERL solar cell invented

$4/$W_p$ 17%

2005 – Suntech NYSE listing

~$500bn

$0.17/$W_p$ 24%

2023

1965 – Singlet fission identified in anthracene: Singh

1979 – Sensitization of PV: Dexter

2012 – SF efficiency limit : Tayebjee

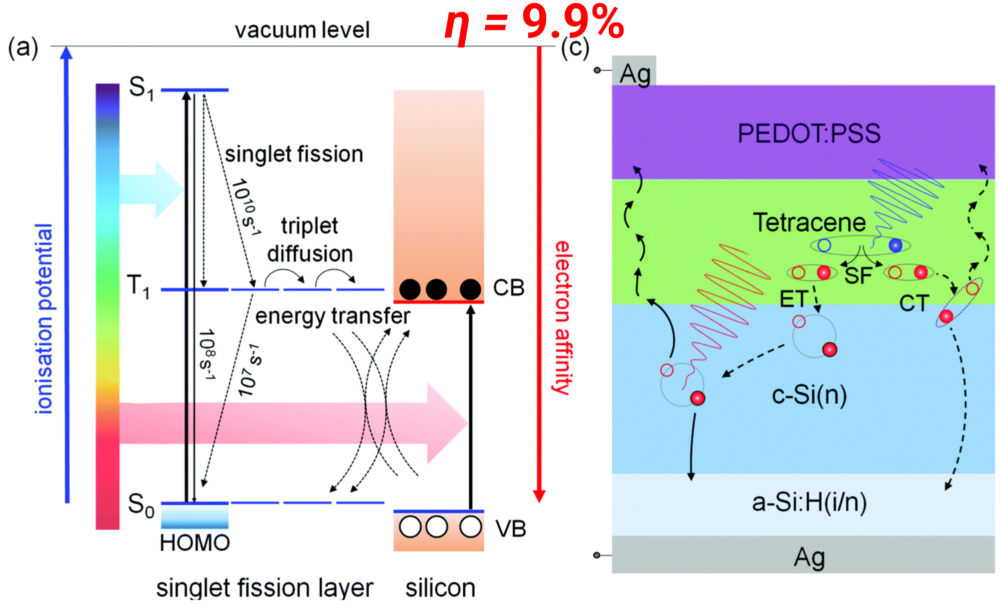
2013 – SF on OPV: Congreve

2019 – SF on silicon: Einzinger

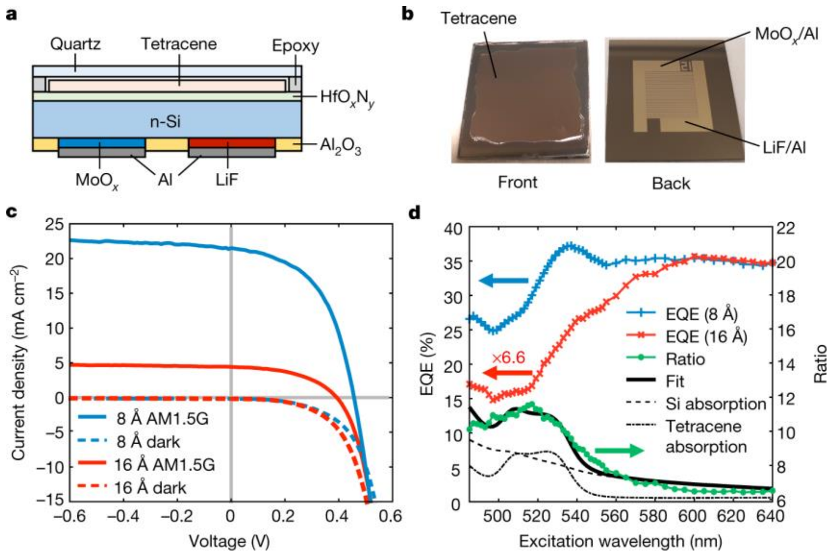
ΩSILICON

Progress

η = 9.9%

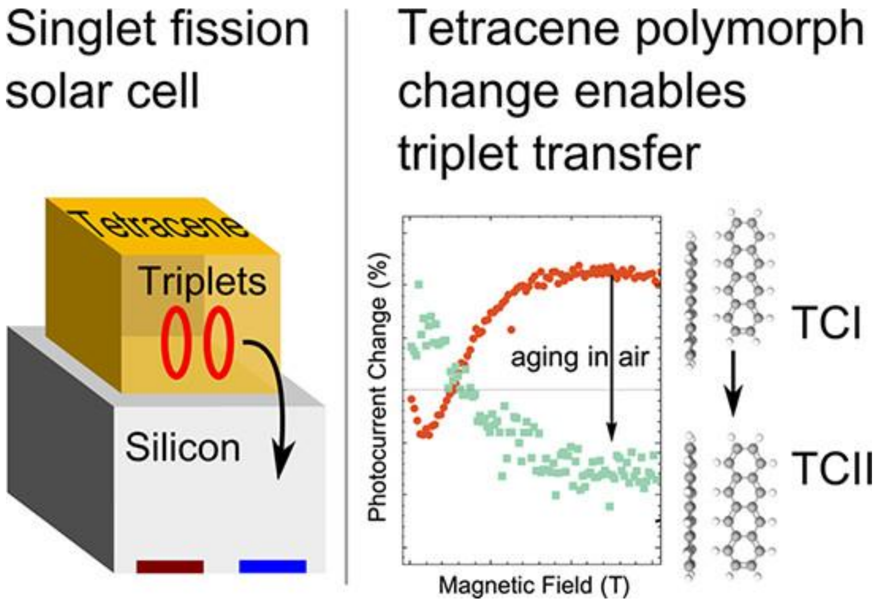


MacQueen, R. W.; Liebhaber, M.; Niederhausen, J.; Mews, M.; Gersmann, C.; Jäckle, S.; Jäger, K.; Tayebjee, M. J. Y.; Schmidt, T. W.; Rech, B.; Lips, K. *Mater Horiz* **2018**, *5* (6), 1065–1075.



η = 5.1%

Einzinger, M.; Wu, T.; Kompalla, J. F.; Smith, H. L.; Perkinson, C. F.; Nienhaus, L.; Wieghold, S.; Congreve, D. N.; Kahn, A.; Bawendi, M. G.; Baldo, M. A. *Nature* **2019**, *571* (7763), 90–94.

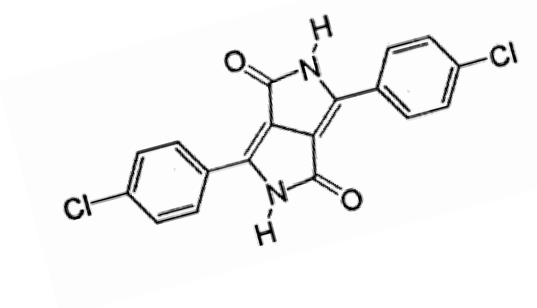


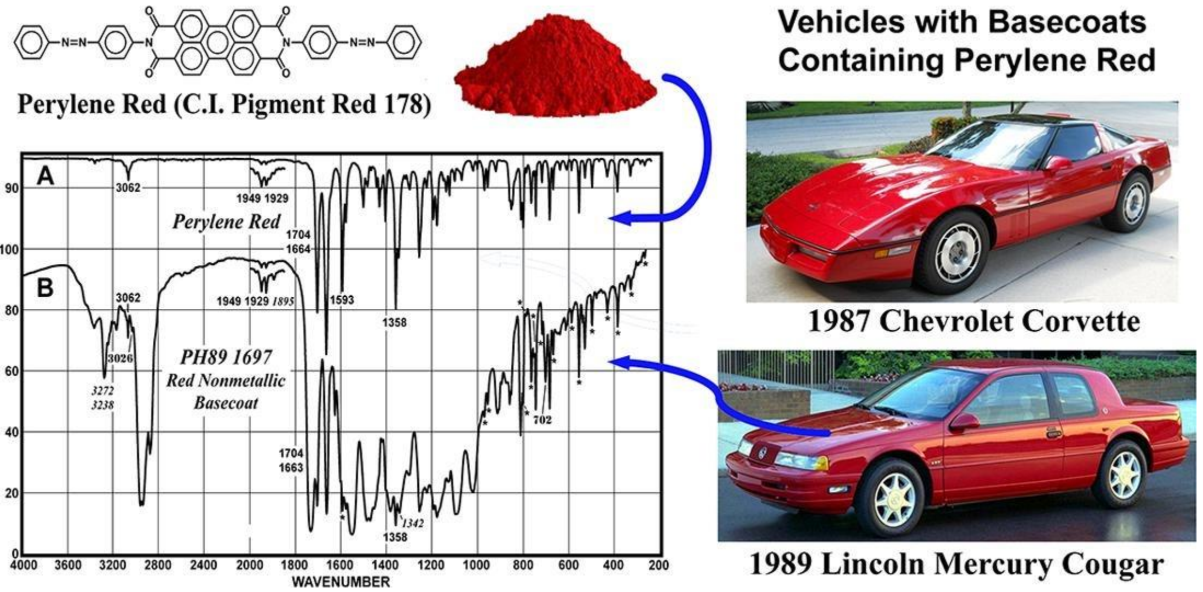
Daiber, B.; Maiti, S.; Ferro, S. M.; Bodin, J.; van den Boom, A. F. J.; Luxembourg, S. L.; Kinge, S.; Pujari, S. P.; Zuilhof, H.; Siebbeles, L. D. A.; Ehrler, B. *J Phys Chem Lett* **2020**, *11* (20), 8703–8709.

Hurdles

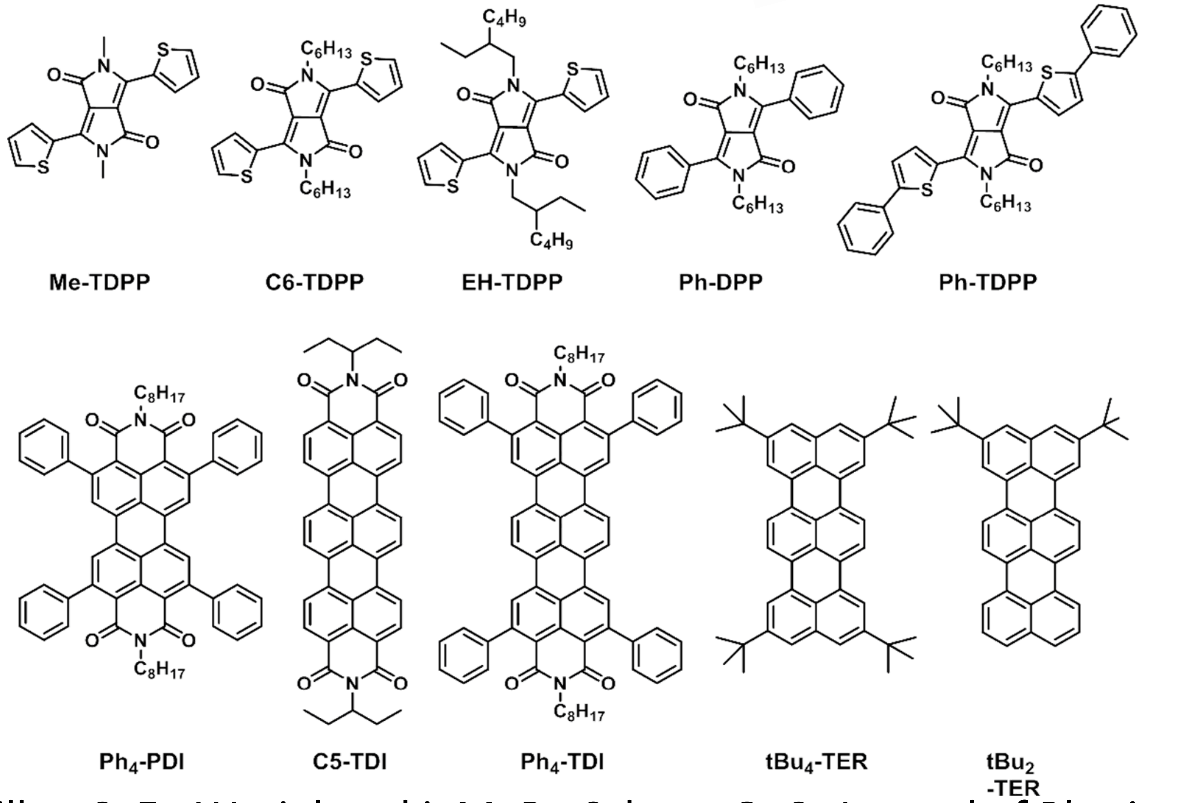
- Stability: ~25 years!
- Parasitic decays of triplets and triplet pairs
  - Rapid singlet fission often gives rapid triplet pair recombination
- Interfaces that both passivate and allow triplet tunneling
  - Thick interfaces passivate
  - Thinner interfaces allow tunneling

Solving Stability



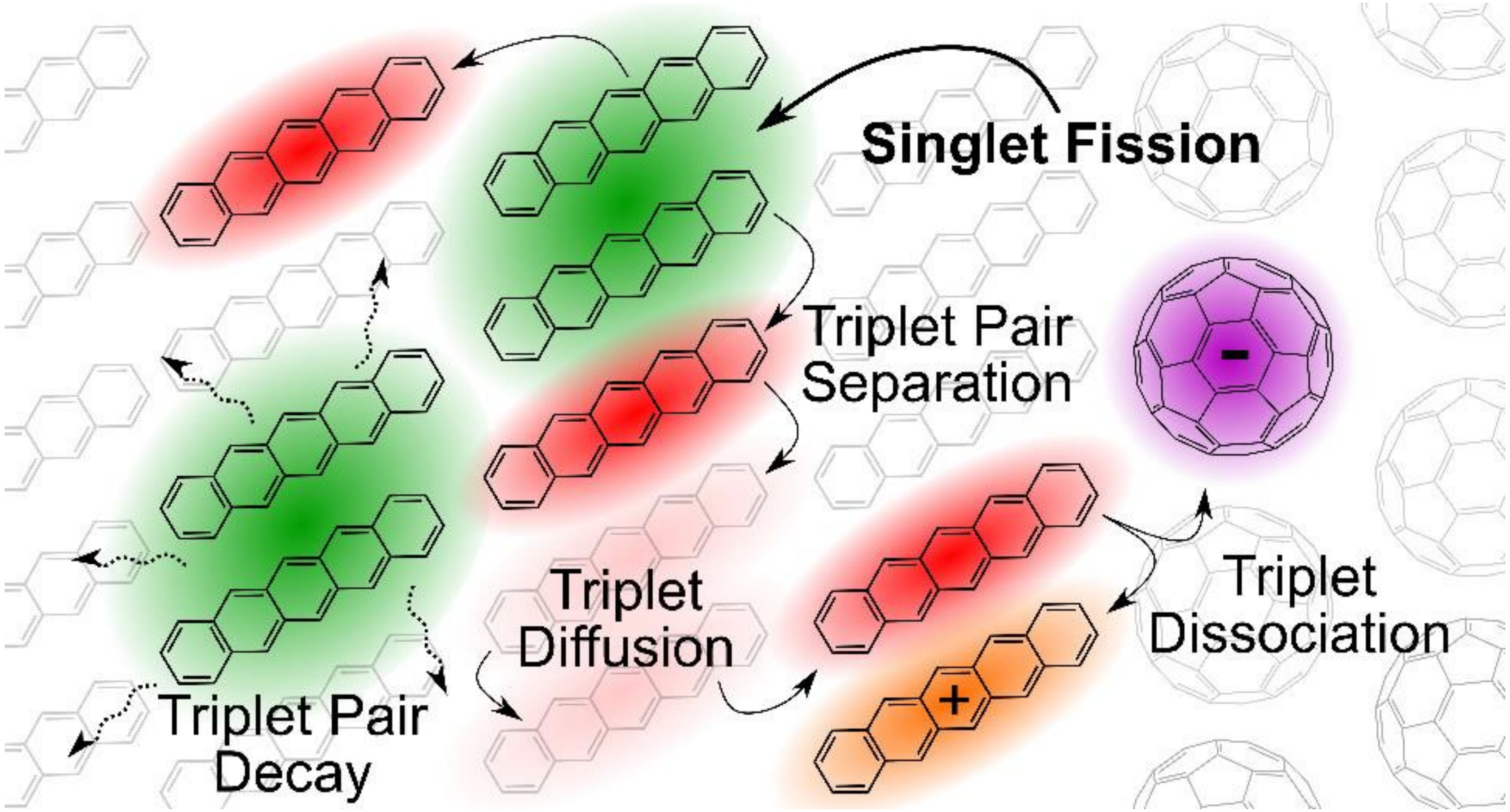


Suzuki, E. M. *Forensic Chemistry* **2022**, *29*, 100420.



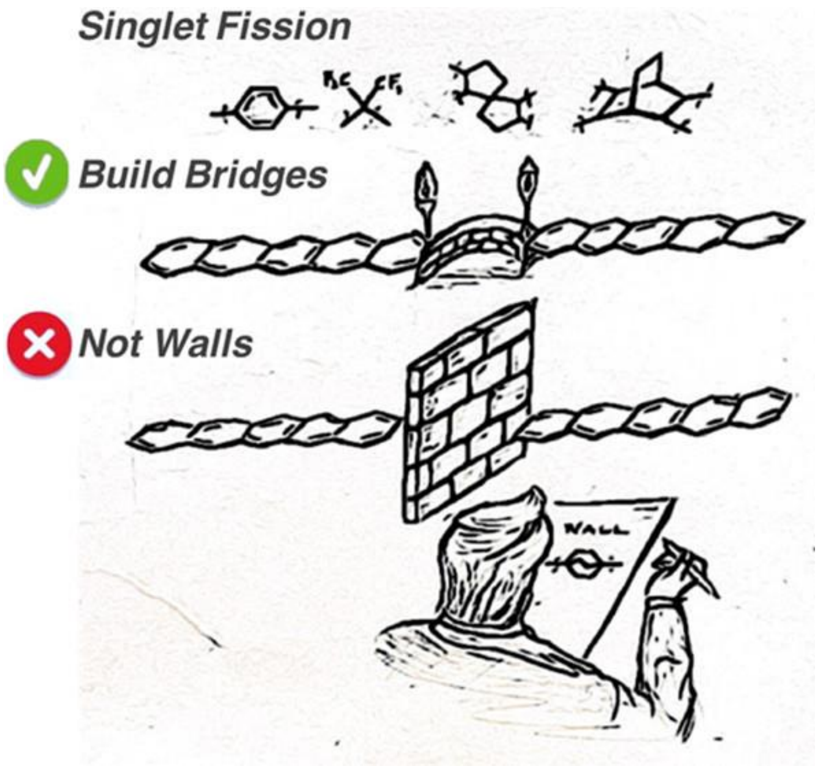
Miller, C. E.; Wasielewski, M. R.; Schatz, G. C. *Journal of Physical Chemistry C* **2017**, *121* (19), 10345–10350.

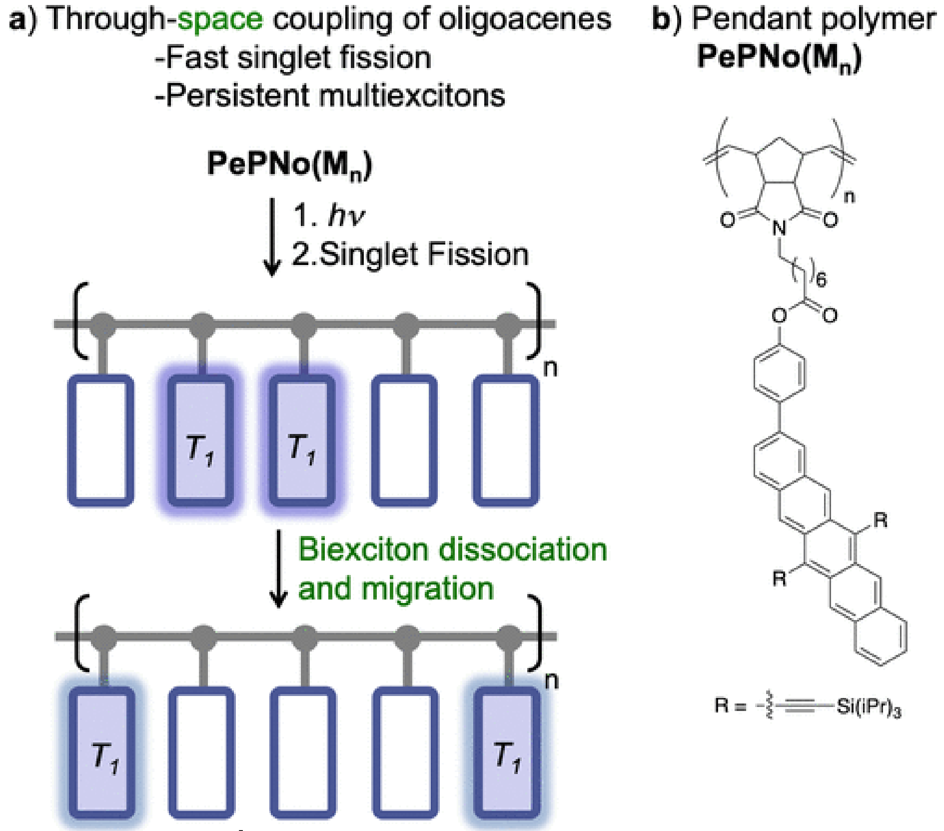
Parasitic Decays



Hudson, R. J.; Stuart, A. N.; Huang, D. M.; Kee, T. W. *The Journal of Physical Chemistry C* **2022**, *126* (12), 5369−5377.

Solving Parasitic Decays

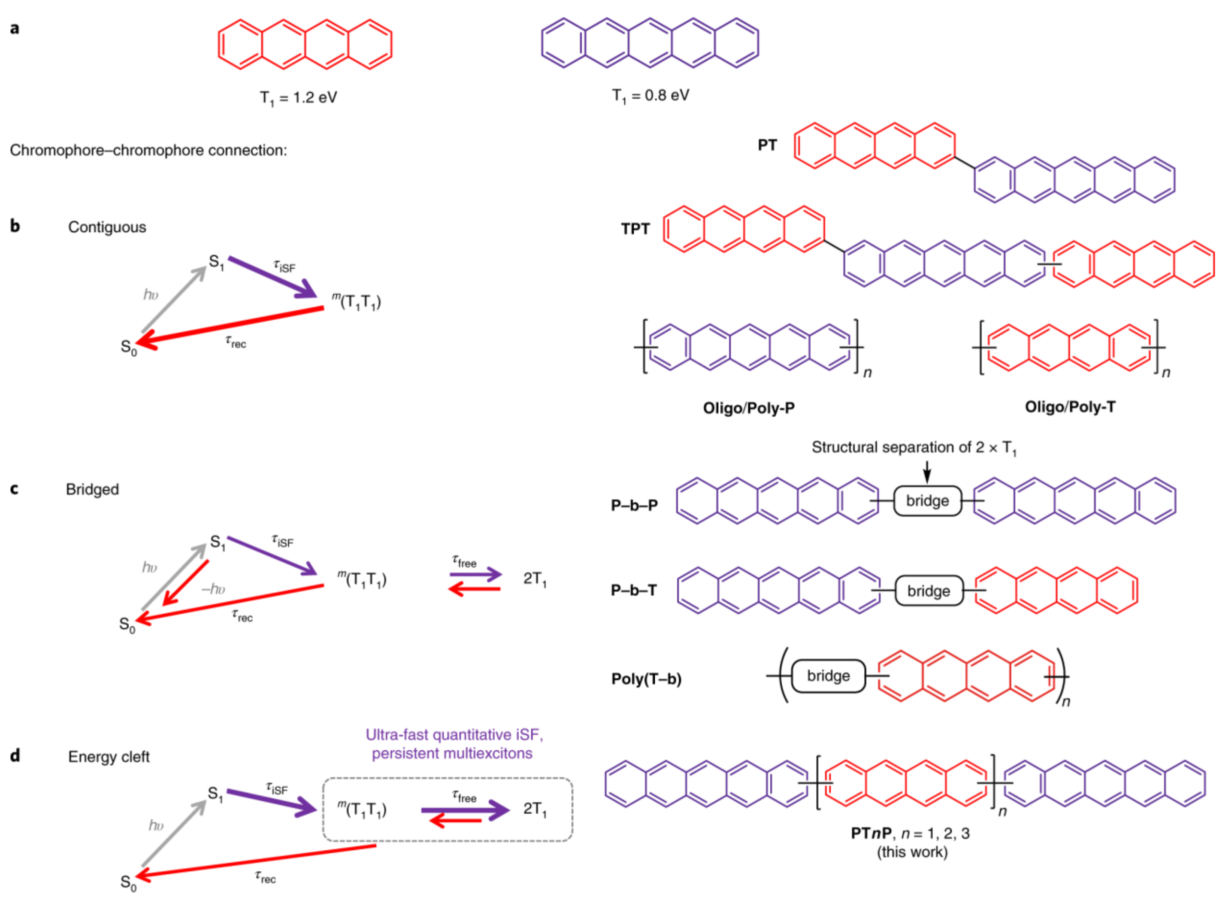




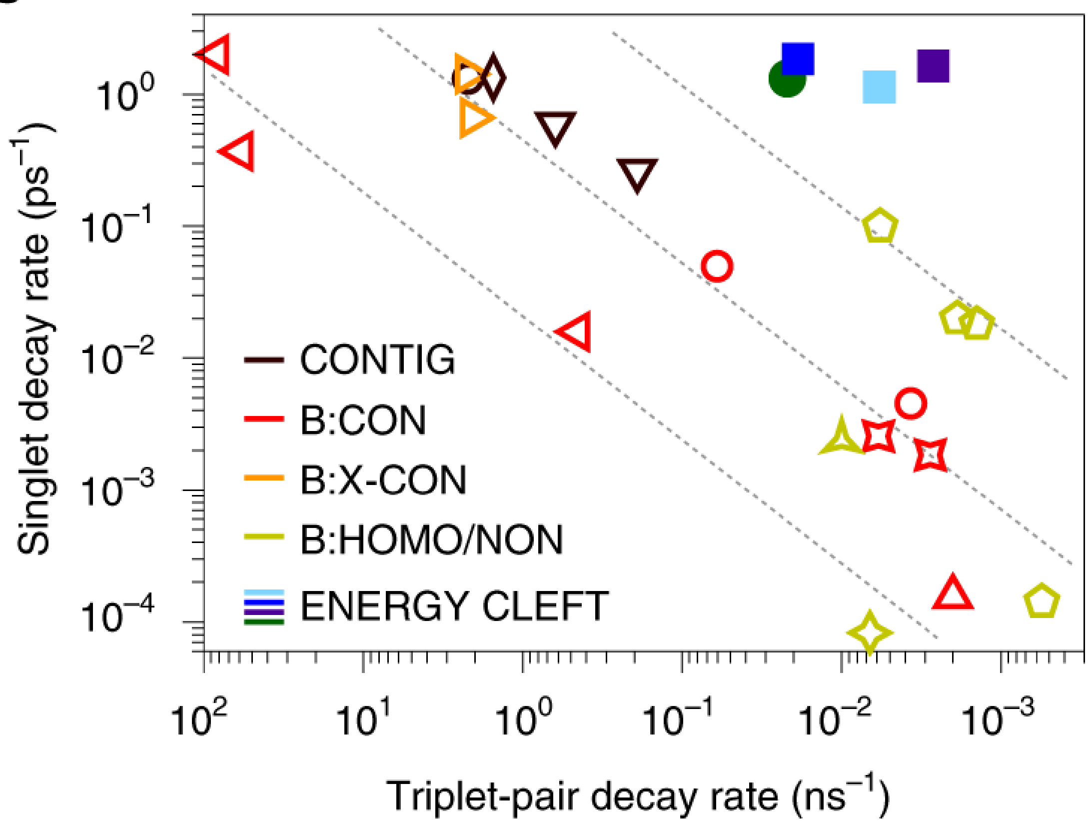
Kumarasamy, E.; Sanders, S. N.; Tayebjee, M. J. Y.; Asadpoordarvish, A.; Hele, J. H.; Fuemmeler, E. G.; Pun, A. B.; Yablon, L. M.; Low, J. Z.; McCamey, D. R.; Sfeir, M. Y.; Campos, L. M. *J Am Chem Soc* **2017**, *139* (36), 12488–12494.

Yablon, L. M.; Sanders, S. N.; Li, H.; Parenti, K. R.; Kumarasamy, E.; Fallon, K. J.; Hore, M. J. A.; Cacciuto, A.; Sfeir, M. Y.; Campos, L. M. *J Am Chem Soc* **2019**, *141* (24), 9564–9569.

Solving Parasitic Decays



b



Pun, A. B.; Asadpoordarvish, A.; Kumarasamy, E.; Tayebjee, M. J. Y.; Niesner, D.; McCamey, D. R.; Sanders, S. N.; Campos, L. M.; Sfeir, M. Y. *Nat Chem* **2019**, *11* (9), 821–828.

Coaxing Triplet Energy into Si

Firstly, how do we know if triplets are making it into Si?

- If we have EQE>100%
- We can use the spin properties of triplets!

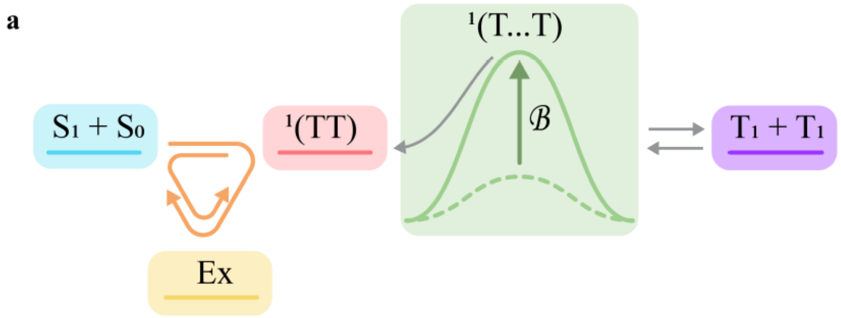


Image by T. W. Schmidt

Coaxing Triplet Energy into Si

Firstly, how do we know if triplets are making it into Si?

- If we have EQE>100%
- We can use the spin properties of triplets!

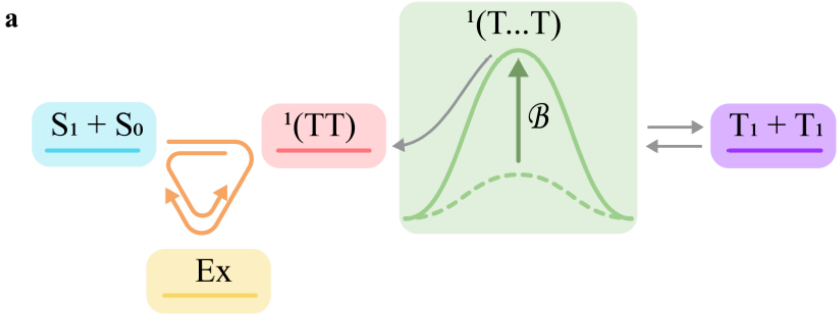
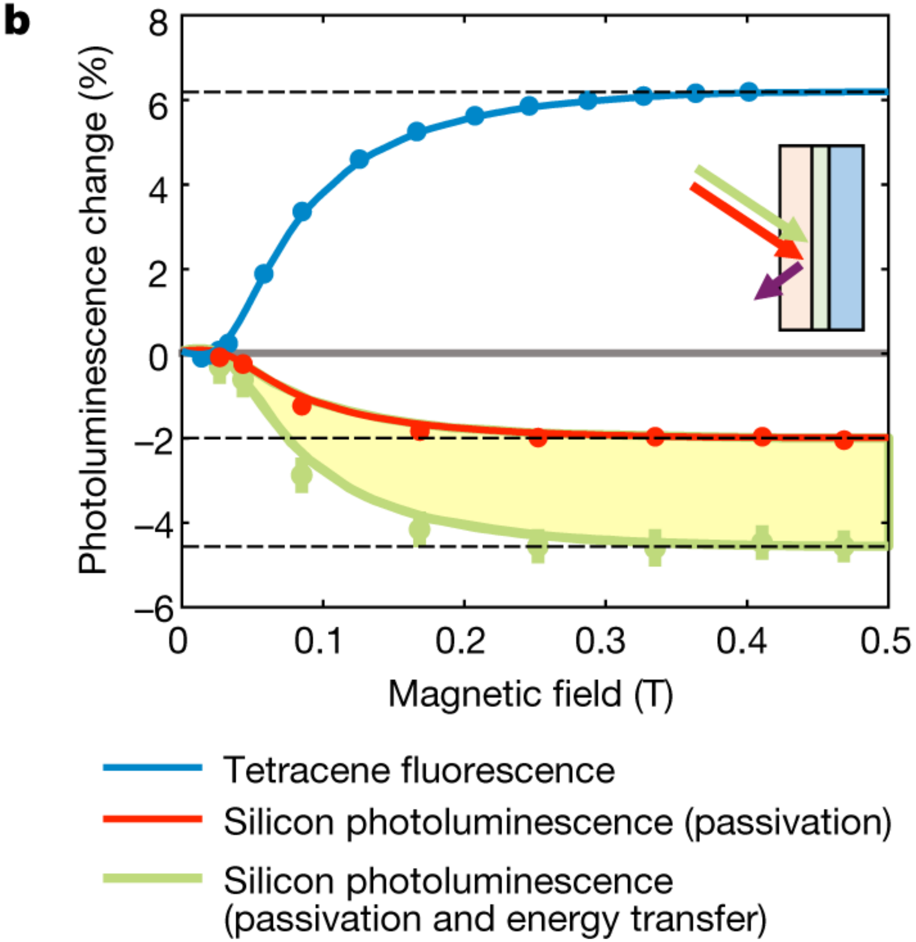
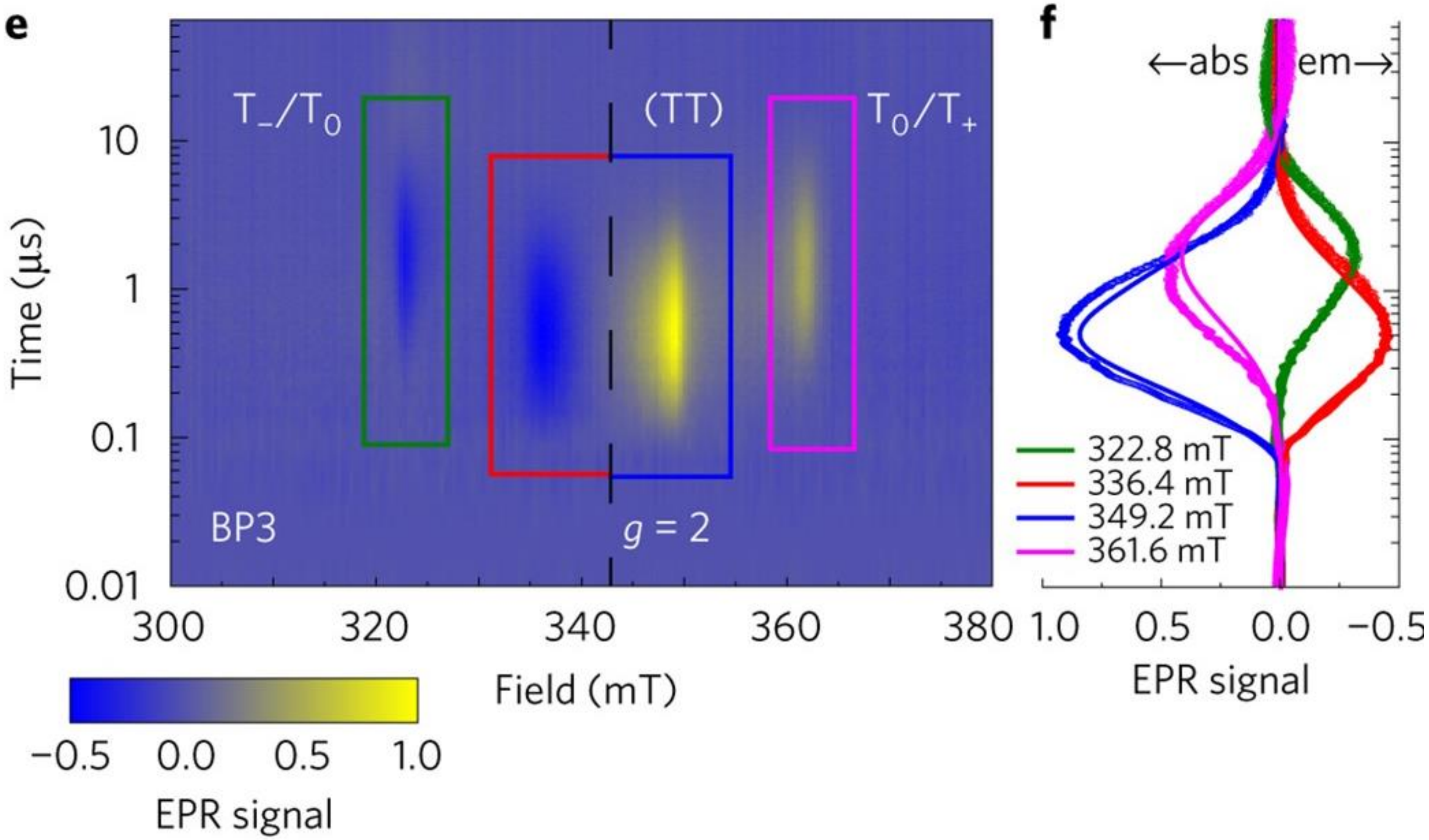


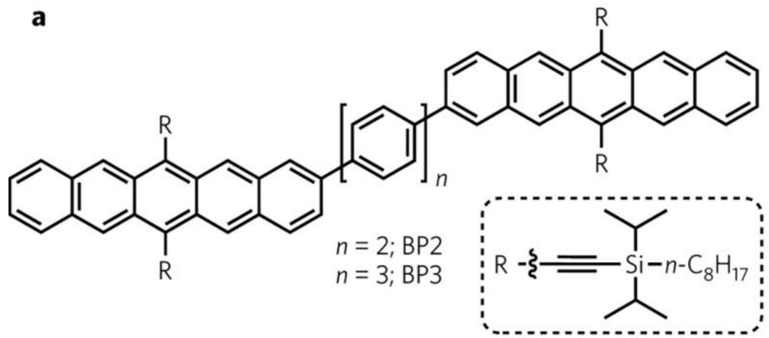
Image by T. W. Schmidt



Einzinger, M.; Wu, T.; Kompalla, J. F.; Smith, H. L.; Perkinson, C. F.; Nienhaus, L.; Wieghold, S.; Congreve, D. N.; Kahn, A.; Bawendi, M. G.; Baldo, M. A. *Nature* **2019**, *571* (7763), 90−94.

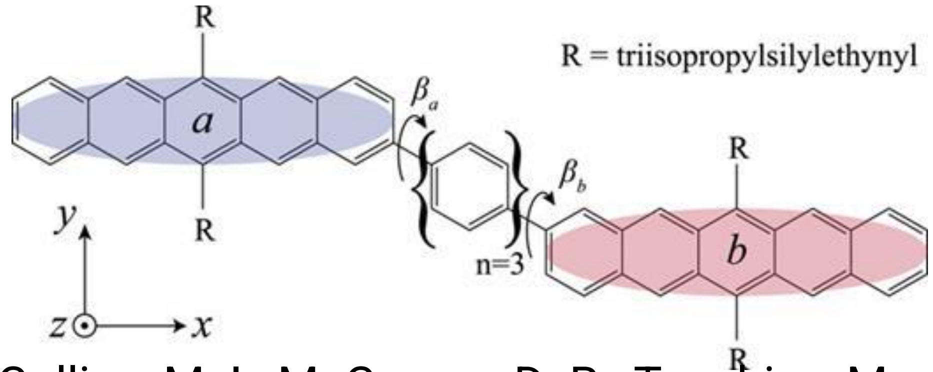
Digression – More than PV!



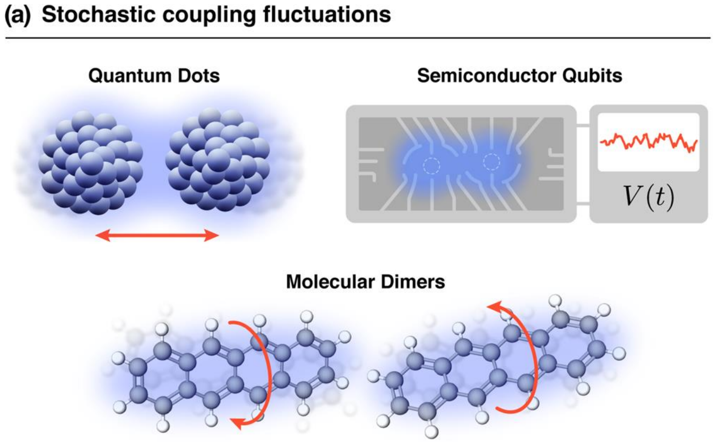


Tayebjee, M. J. Y.; Sanders, S. N.; Kumarasamy, E.; Campos, L. M.; Sfeir, M. Y.; McCamey, D. R. *Nat Phys* **2017**, *13* (2), 182–188.

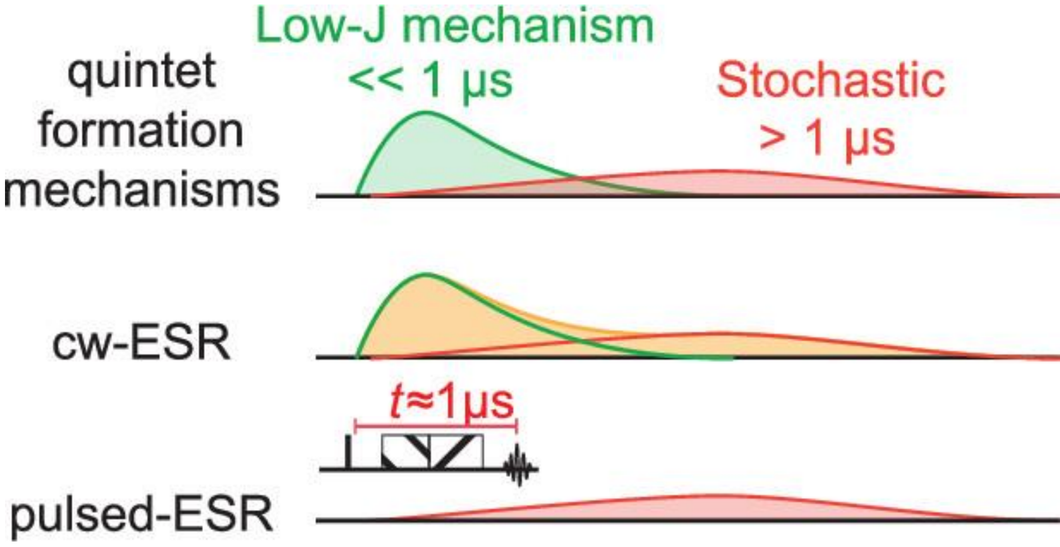
Digression – more than PV!



Collins, M. I.; McCamey, D. R.; Tayebjee, M. J. Y. *J Chem Phys* **2019**, *151* (16), 164104.

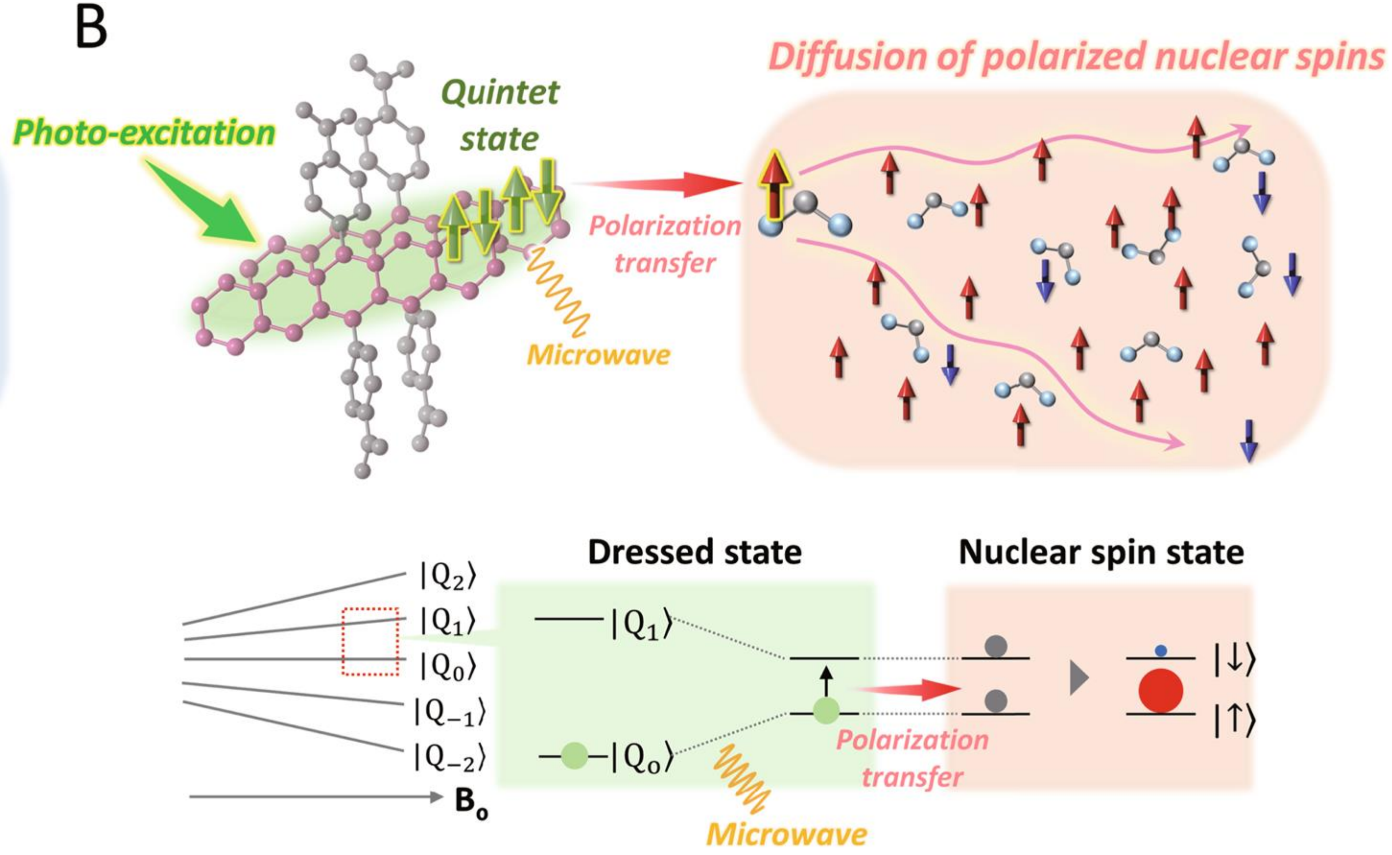


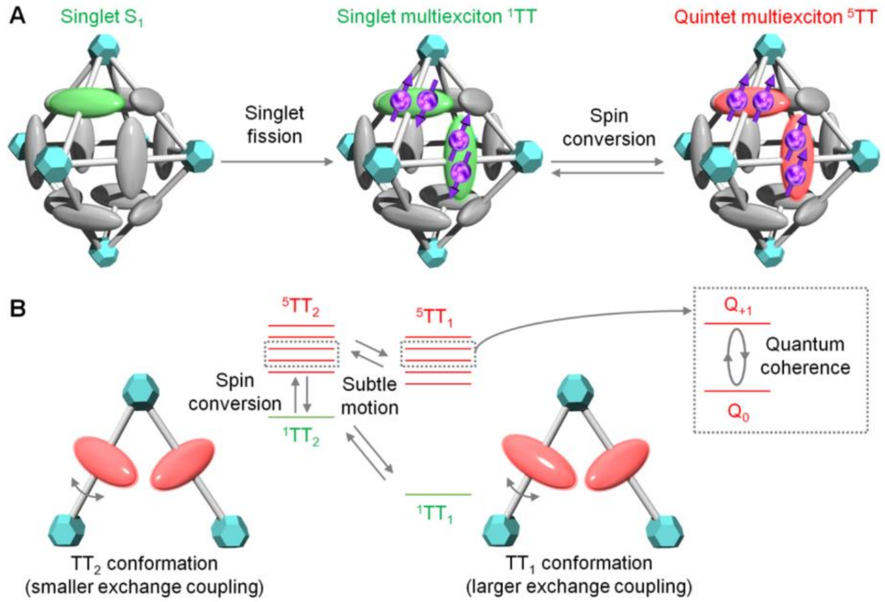
Collins, M. I.; Campaioli, F.; Tayebjee, M. J. Y.; Cole, J. H.; McCamey, D. R. *Commun Phys* **2023**, *6* (1), 64.



MacDonald, T. S. C.; Tayebjee, M. J. Y.; Collins, M. I.; Kumarasamy, E.; Sanders, S. N.; Sfeir, M. Y.; Campos, L. M.; McCamey, D. R. *J Am Chem Soc* **2023**, *145* (28), 15275–15283.

Digression – more than PV!

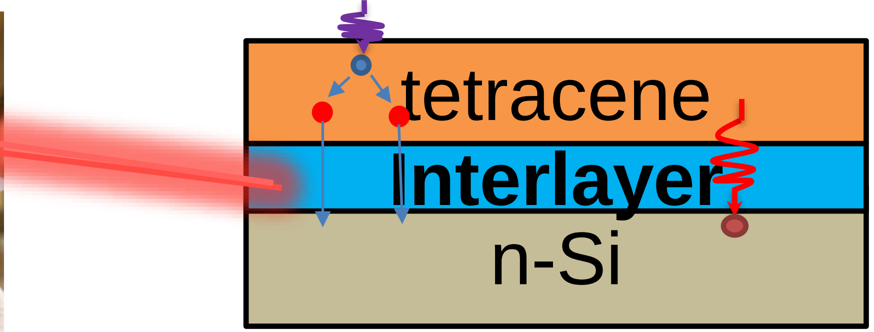


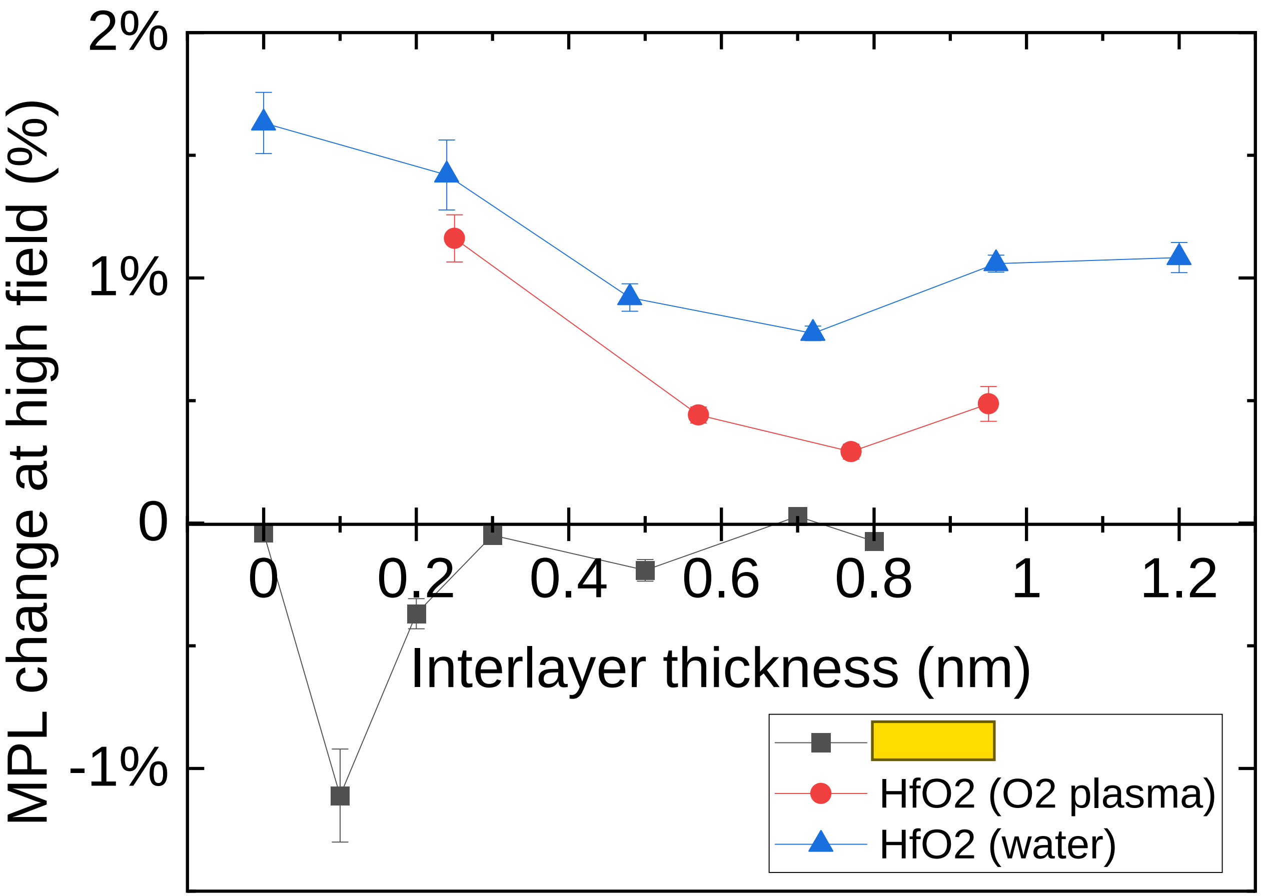


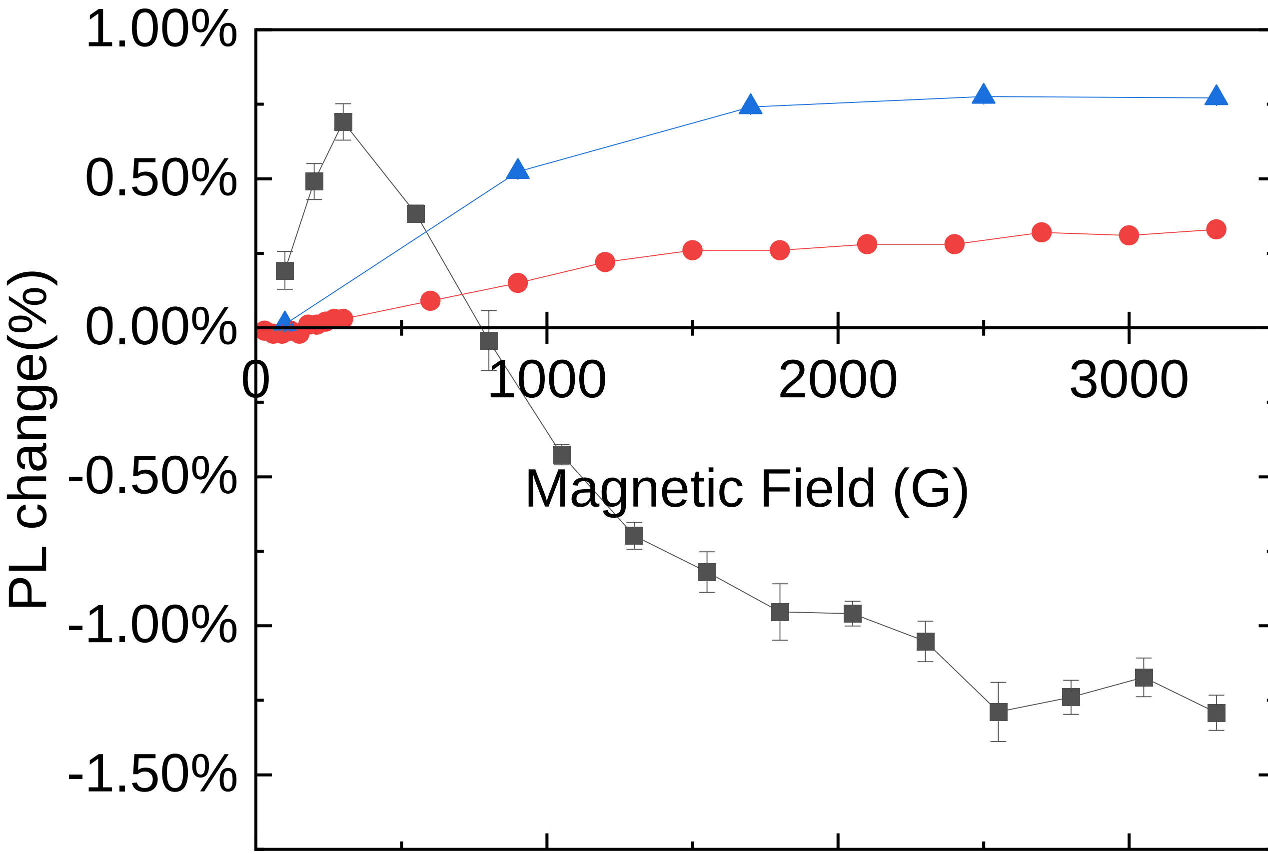
10.26434/chemrxiv-2023-nz6rz

Kawashima, Y.; Hamachi, T.; Yamauchi, A.; Nishimura, K.; Nakashima, Y.; Fujiwara, S.; Kimizuka, N.; Ryu, T.; Tamura, T.; Saigo, M.; Onda, K.; Sato, S.; Kobori, Y.; Tateishi, K.; Uesaka, T.; Watanabe, G.; Miyata, K.; Yanai, N. *Nat Commun* **2023**, *14* (1), 1056.

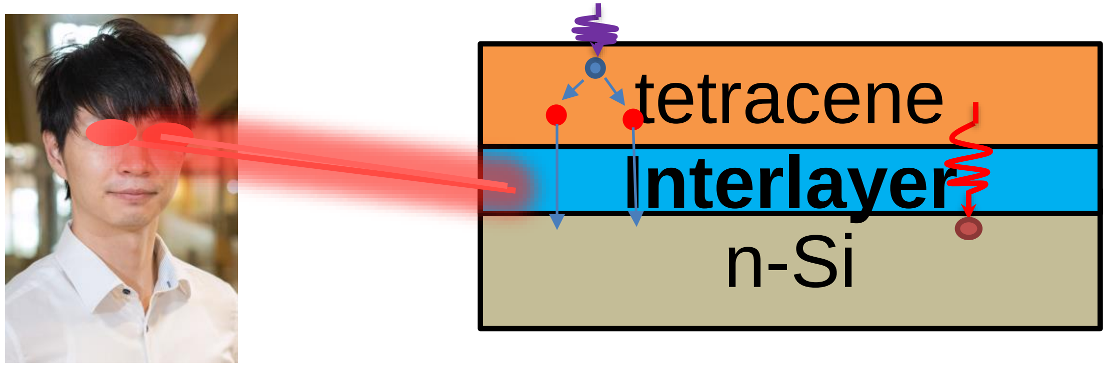
Results from our lab

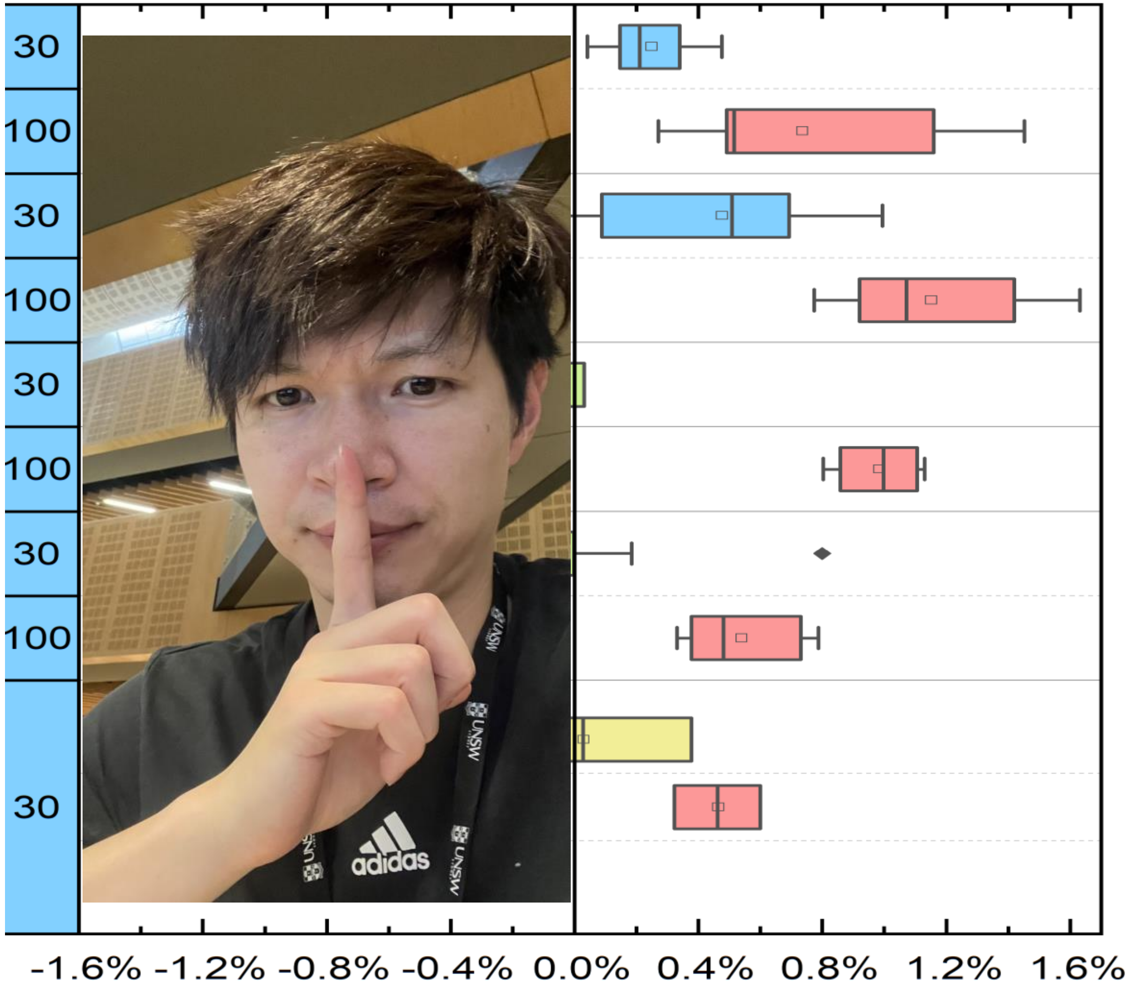






Results from our lab





Conclusions

- ΩSi allows us to circumvent many of the challenges of conventional silicon tandems,
- But… it also introduces a few!
- We have three big hurdles
- But… We have more than three solutions!

DASOLAR 一道新能
JA SOLAR
Xinhao Energy
阿特斯
JinKO Solar
Leadmicro 微导
JINERGY
中来股份 JOLYWOOD
ARENA Australian Government Australian Renewable Energy Agency
MSCA
Australian Government Australian Research Council