

# Centre for Advanced Materials for Integrated Energy Systems (CAM-IES)

Kick Off meeting – January 2017

**WP4 Organic-inorganic hybrid interfaces -  
Spin triplet excitons for photovoltaics.**

WP4 Leader: Hugo Bronstein - UCL

# Members

## UCL

*Bronstein – WP Leader, Synthesis*

*Cacialli – Devices, photophysics*

*Clarke - Spectroscopy*

*Papakonstantinou - Characterization*

## CAM

*Friend – Spectroscopy, Devices*

*Greenham – Spectroscopy, Nanocrystals*

*Rao – Spectroscopy, Devices*

## QMUL

*Nielsen - Synthesis*

*Gillin – Characterization, Spin*

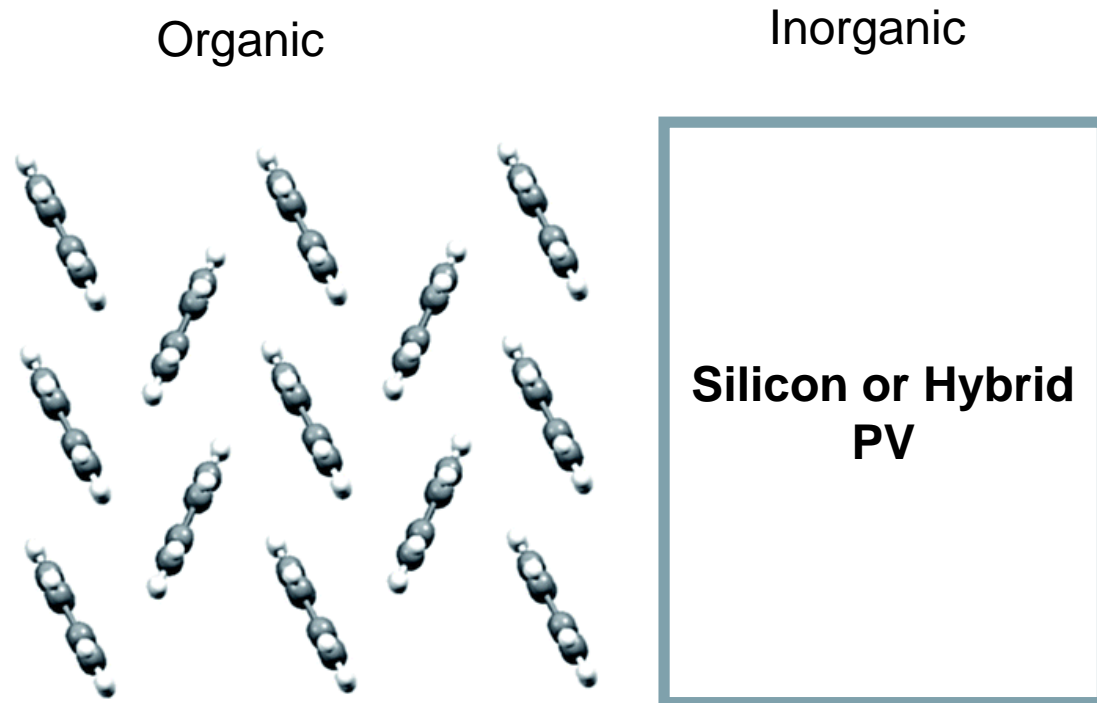
## NCU

*Gibson – Photo/electro chemistry*

*Penfold – Simulation, Theory*

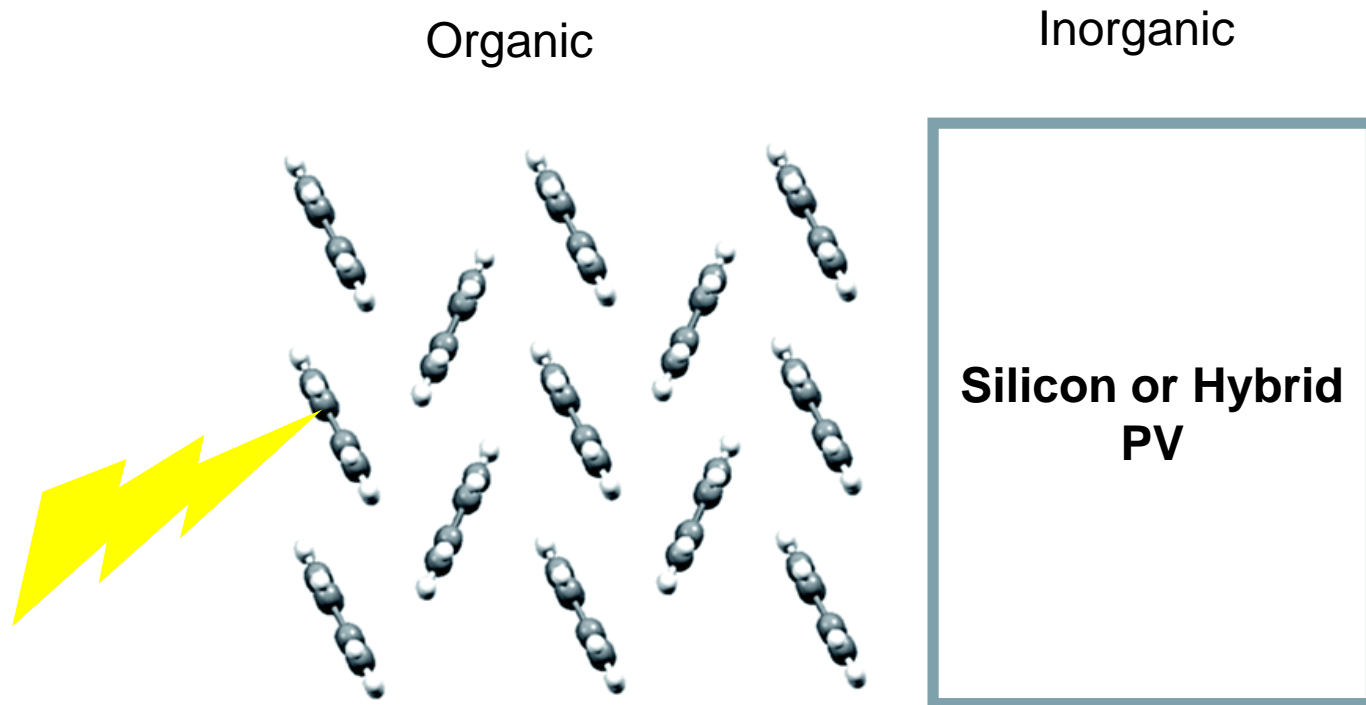
*Cucinotta – Supramolecular chemistry*

# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics



**AIM: Increase the efficiency of inorganic PV through the use of Singlet Fission**

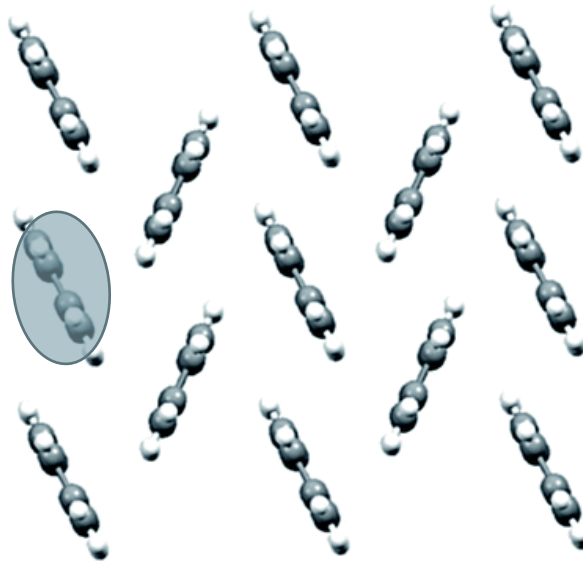
# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics



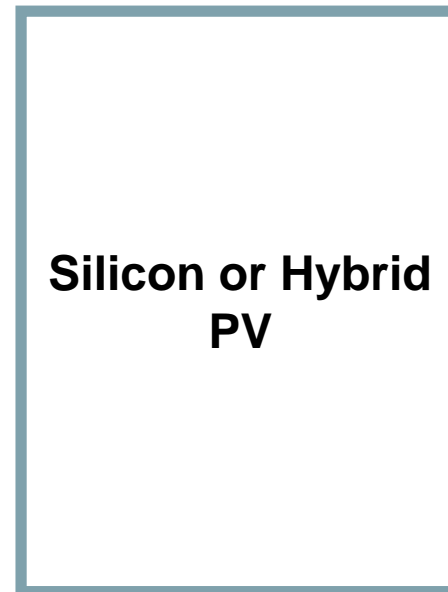
**1. Light Absorption**

# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics

Organic



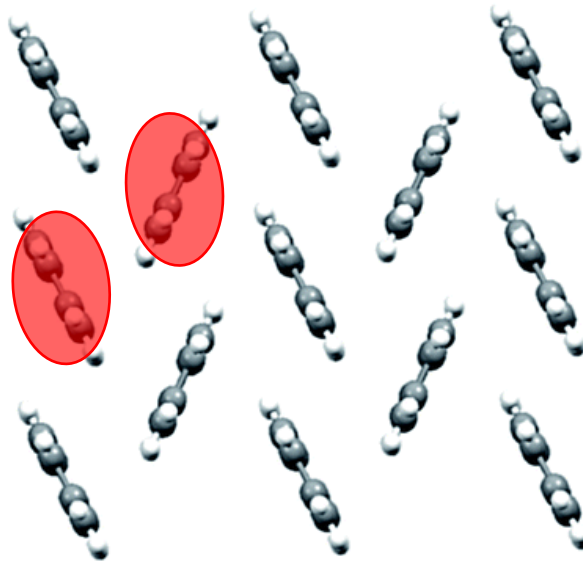
Inorganic



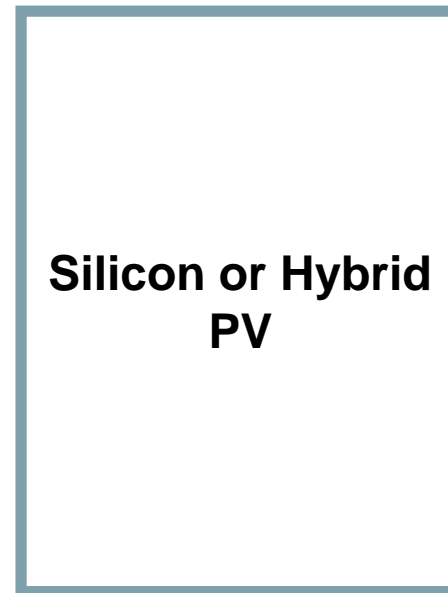
## 2. Singlet Formation

# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics

Organic

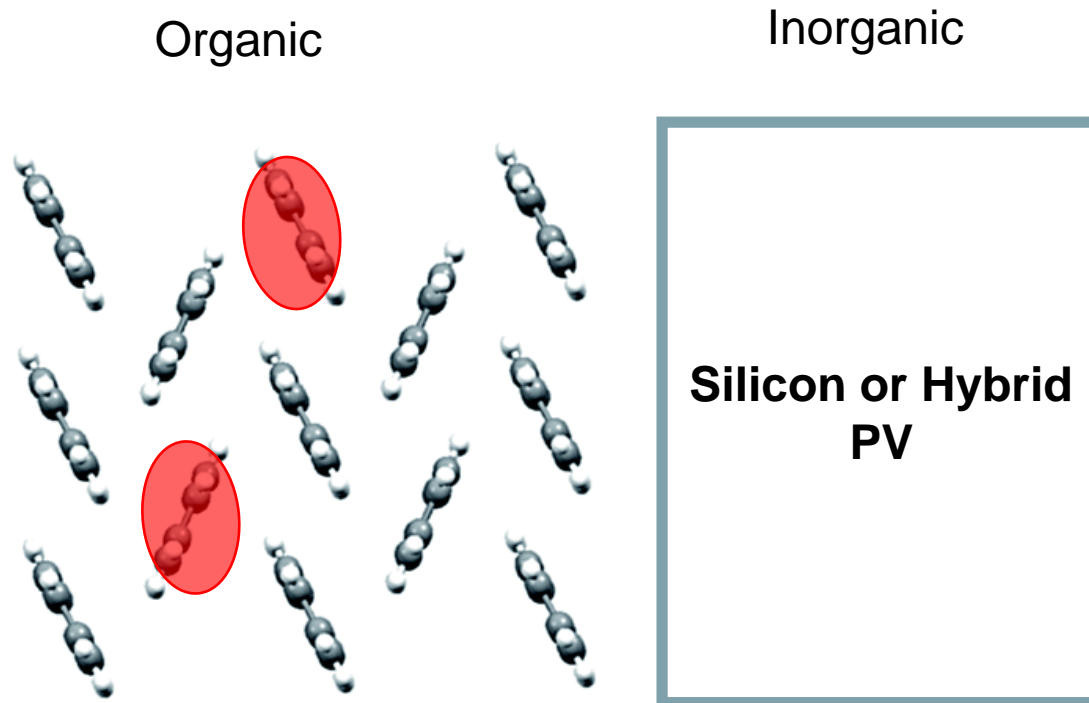


Inorganic



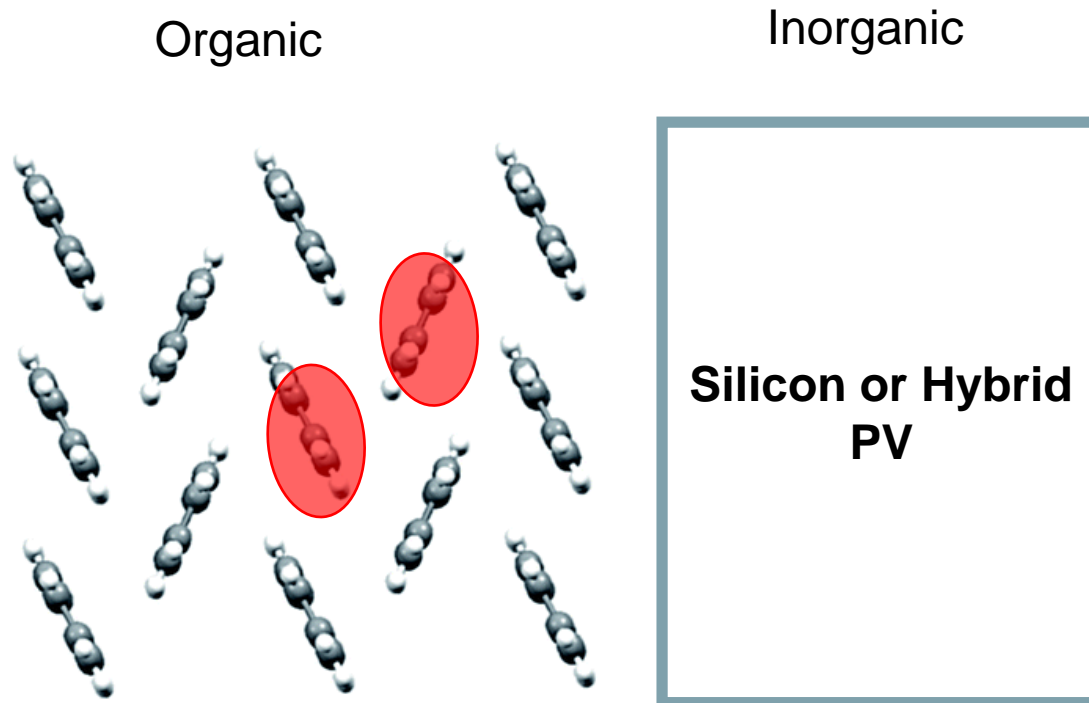
## 3. Singlet Fission

# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics



## 4. Triplet Diffusion

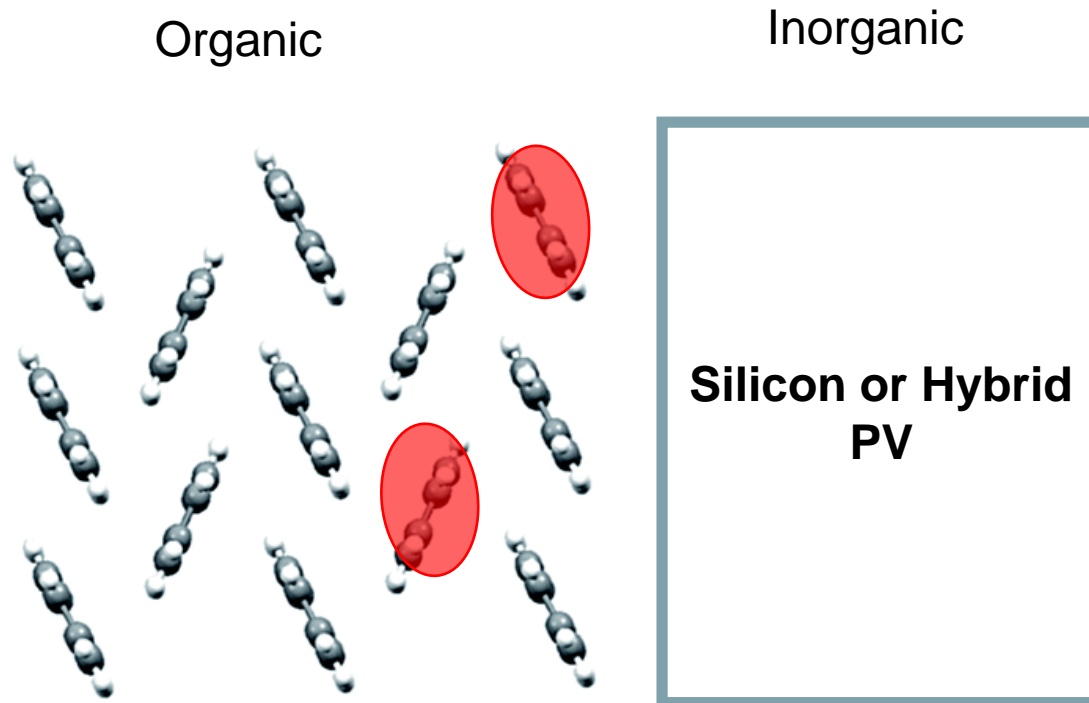
# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics



## 4. Triplet Diffusion

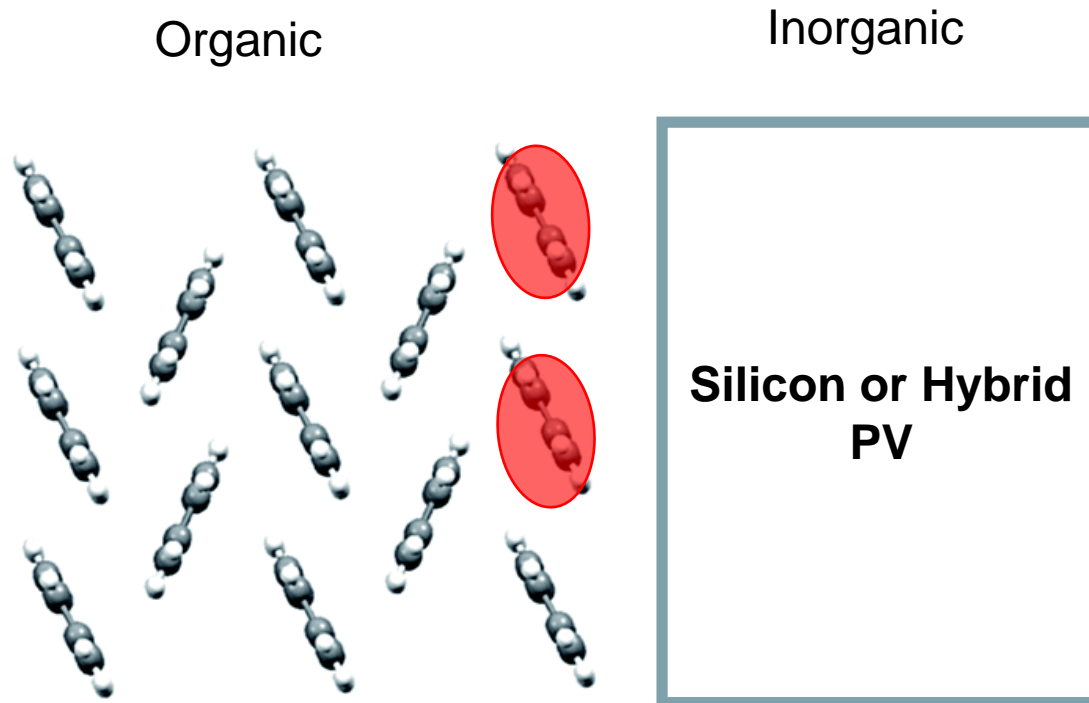


# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics



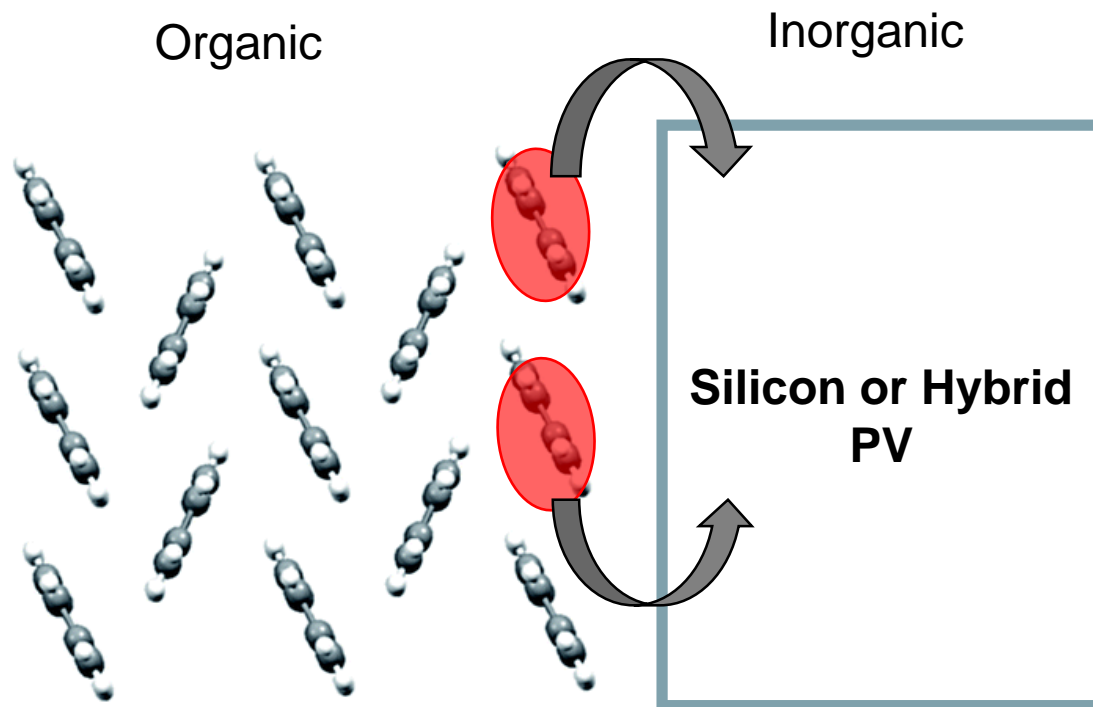
## 4. Triplet Diffusion

# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics



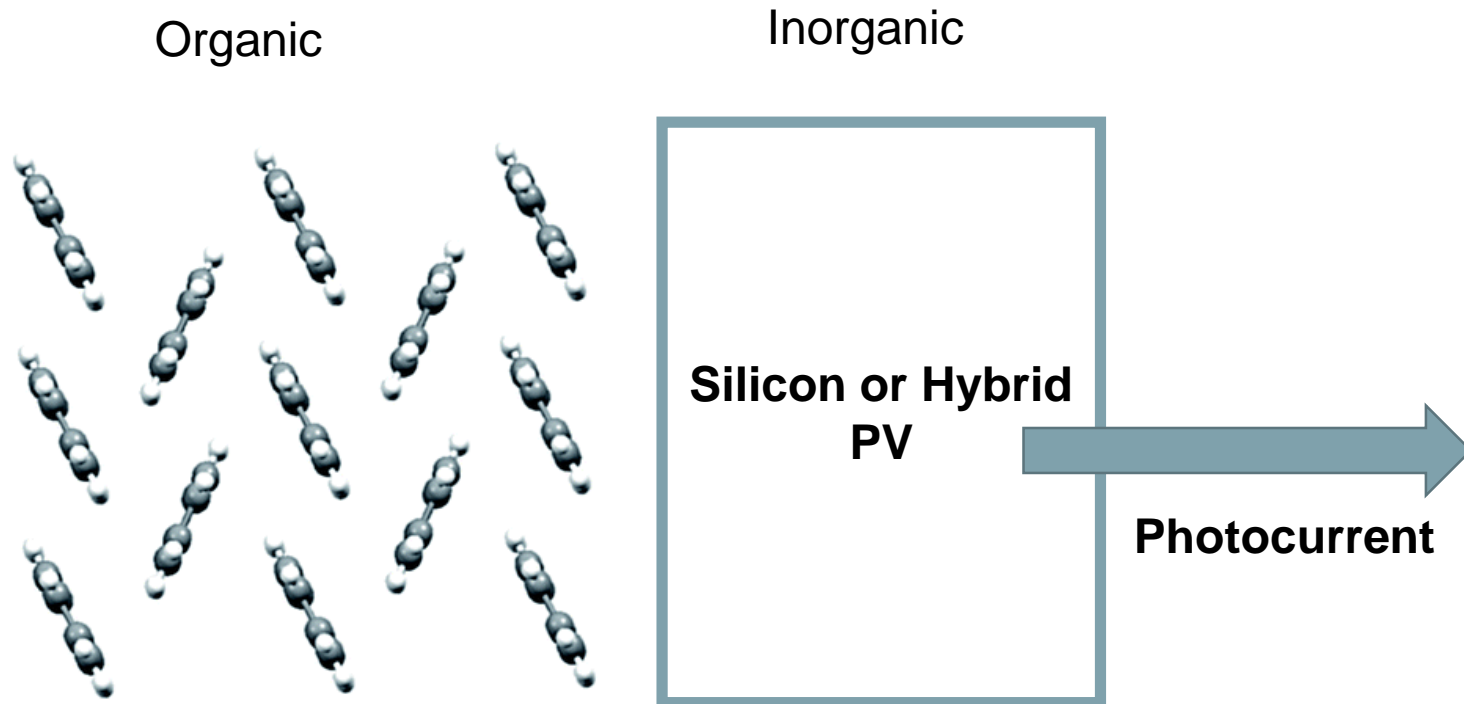
## 4. Triplet Diffusion

# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics



## 5. Triplet Injection

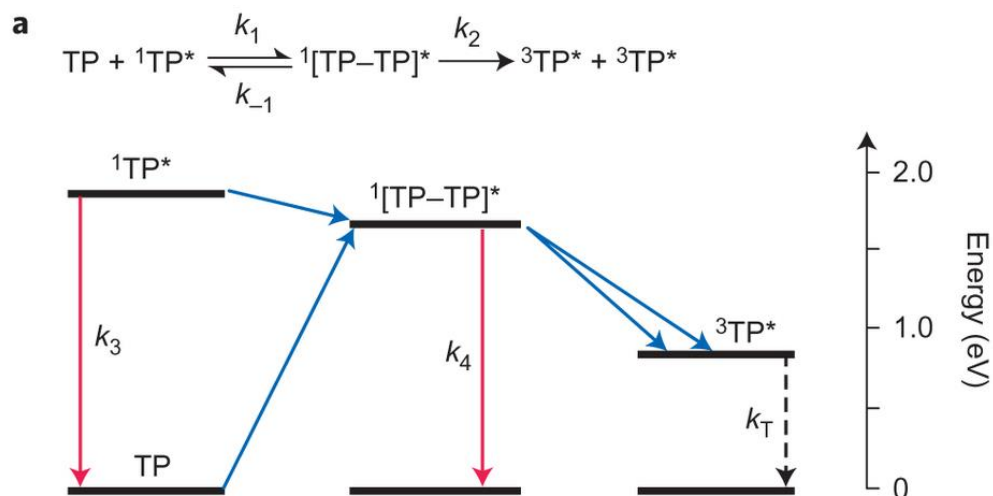
# Organic-inorganic hybrid interfaces - Spin triplet excitons for photovoltaics



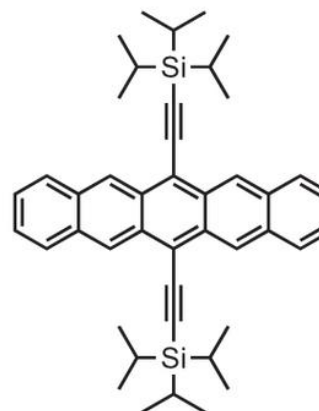
## 6. Photocurrent Generation

# 1+2+3. Light Absorption/Singlet Fission

Singlet Fission has very strict energetic requirements



TIPS-pentacene (TP)



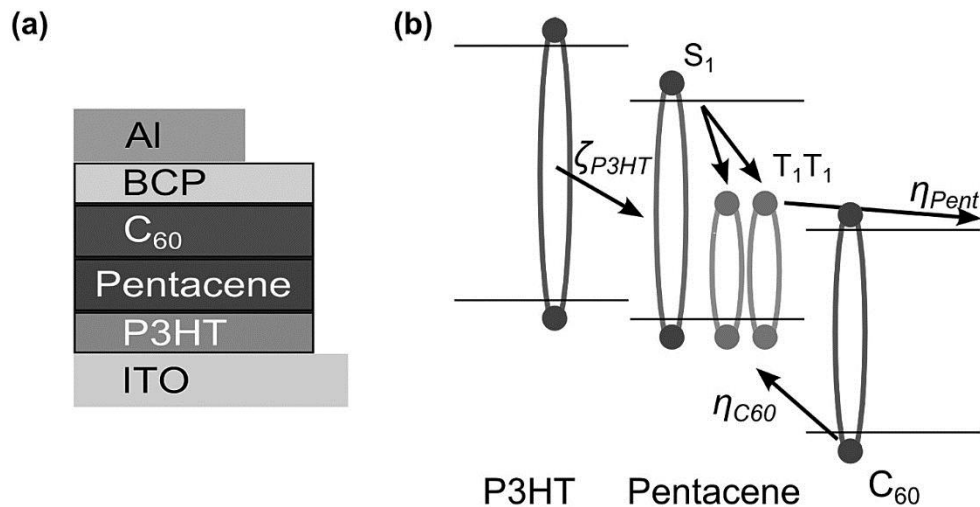
Brian J. Walker, Andrew J. Musser, David Beljonne, Richard H. Friend, *Nature Chemistry* 5, 1019–1024 (2013)

Linear acenes (tetracene, pentacene) almost exclusively used  
Suffer from poor stability and lack of tunability (limits choice of inorganic component)

**TASK: Develop stable, tunable materials for singlet fission (UCL-CAM)**

## 4. Triplet Diffusion

Triplet diffusion in organic materials is not well understood.  
 Large range of values ranging from  $\sim 0$  (immobile) to 2 microns.



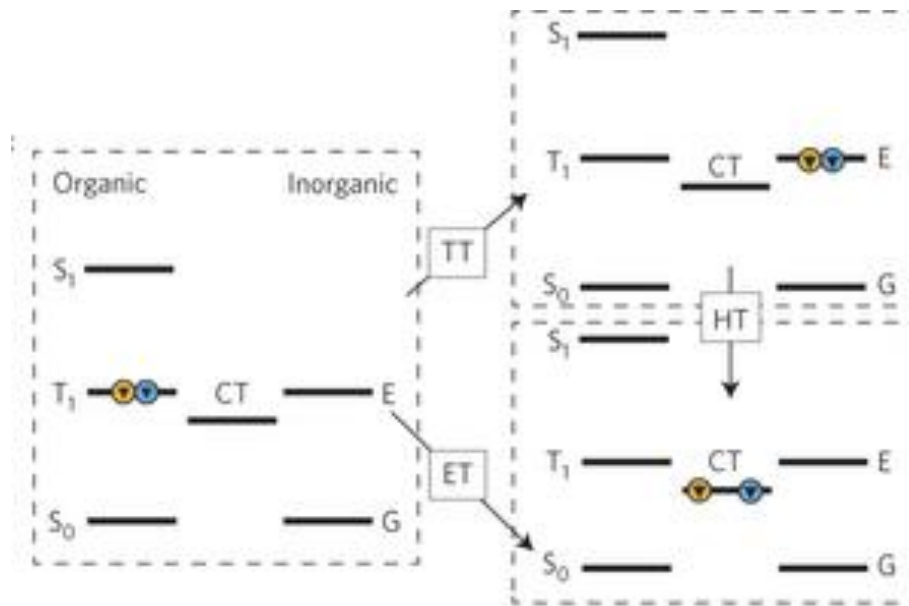
Triplet exciton diffusion in pentacene (a singlet fission material) found to be 40 nm.

Maxim Tabachnyk, Bruno Ehrler, Sam Bayliss, Richard H. Friend, and Neil C. Greenham, Applied Physics Letters 2013 103:15

***TASK: Develop understanding of triplet diffusion in organic materials (i.e diffusion anisotropy, effect of morphology, exciton confinement etc..) (UCL)***

# 5. Triplet Injection

Direct injection of triplet excitons into an inorganic semiconductor has only recently been demonstrated from pentacene to PbSe



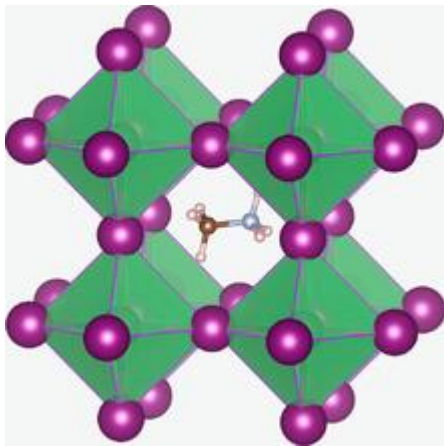
Efficient transfer seems to require resonance ( $\pm 0.2$  eV) of the triplet energy with the bandgap of the inorganic semiconductor.

Effect of molecular orientation, distance, interlayers and energetics almost completely unexplored

Maxim Tabachnyk, Bruno Ehrler, Simon Gélinas, Marcus L. Böhm, Brian J. Walker, Kevin P. Musselman, Neil C. Greenham, Richard H. Friend, Akshay Rao, Nature Materials 13, 1033–1038 (2014)

***TASK: Develop an understanding the nature of the interface between organic and inorganic semiconductors with an aim to increasing triplet injection (CAM)***

## 6. Choice of Inorganic Semiconductor/Photocurrent Generation



Perovskite solar cells are of comparable efficiency to Silicon PV, and there are numerous other potential inorganic materials (eg ZnO, PbSe etc..). Each have their benefits and drawbacks.

Important to understand the generality of the inorganic-organic interface with different semiconductors. Also, possibility of chemical modification of some of these to directly link organic-inorganic components

***TASK: Determine optimum inorganic materials for interface. Explore the possibility of surface modifications/functionalisation. (CAM)***



**Looking Forward to It!**