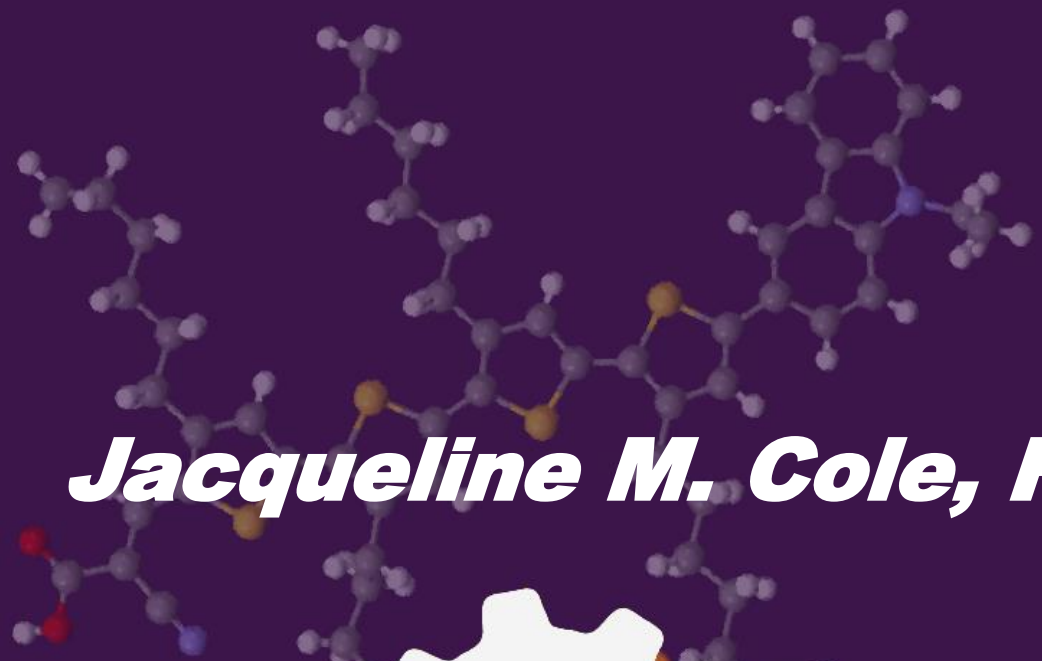
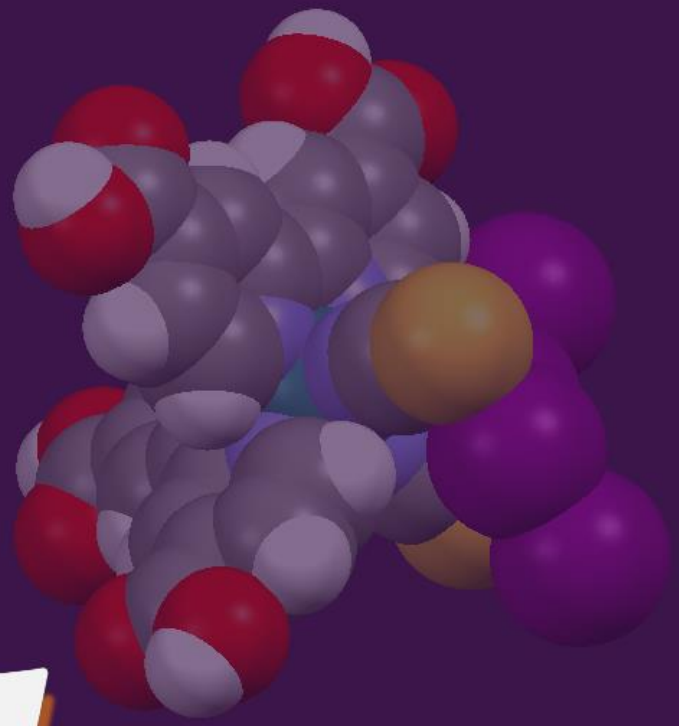




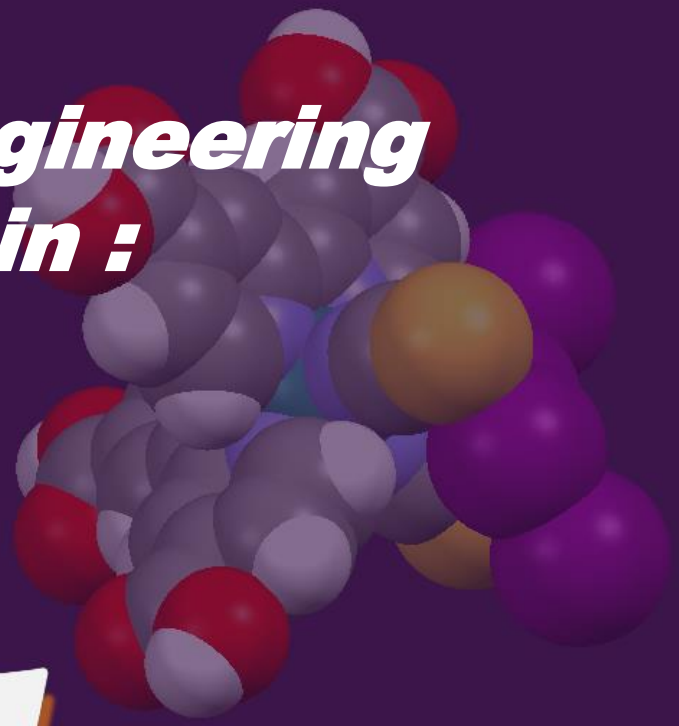
*Jacqueline M. Cole, Head*

# Molecular Engineering

*A partnership between Cambridge University, BASF & STFC RAL*

**BASF / Royal Academy of Engineering**
**Senior Research Fellowship in :**

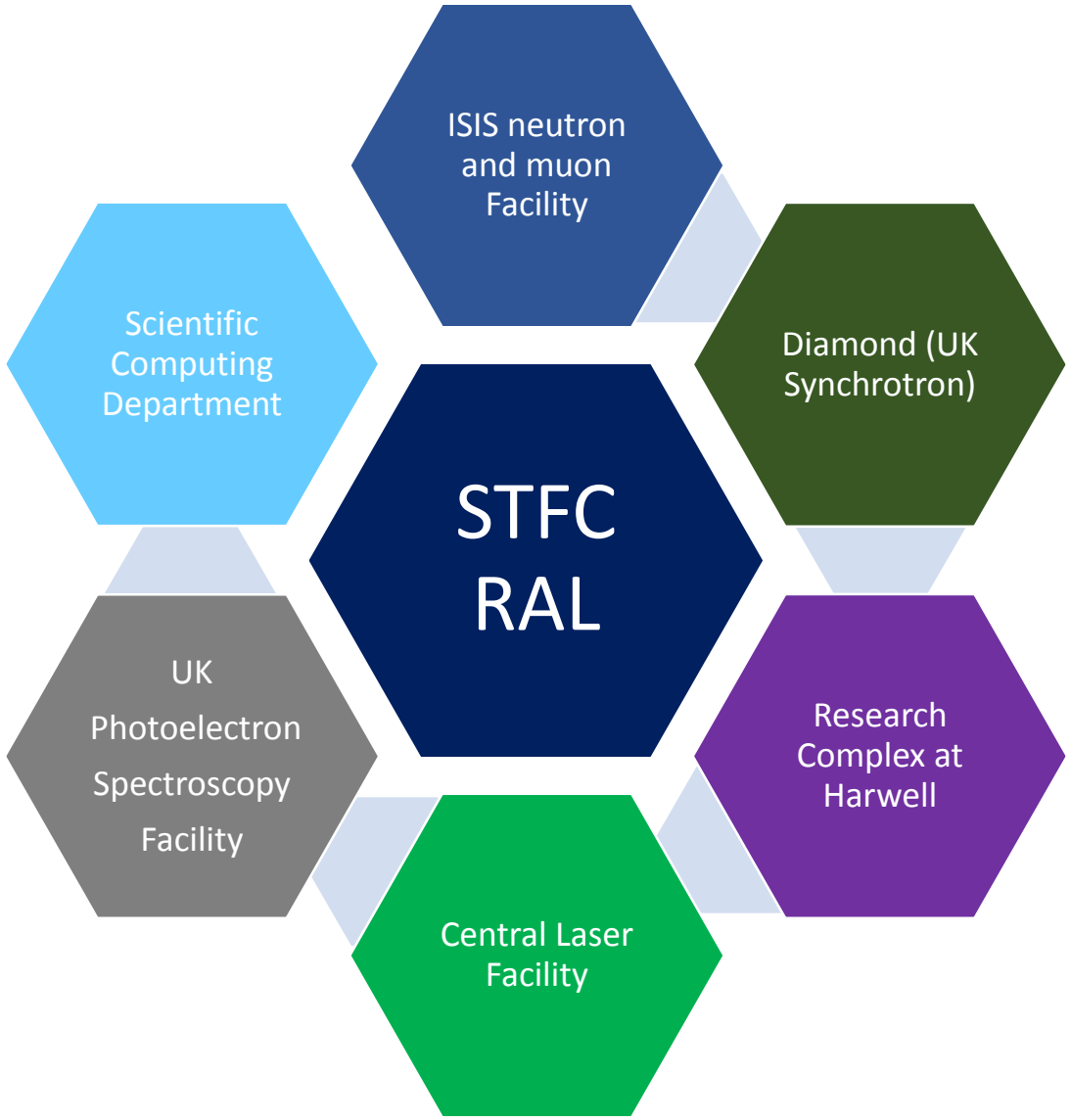
**Data Driven**



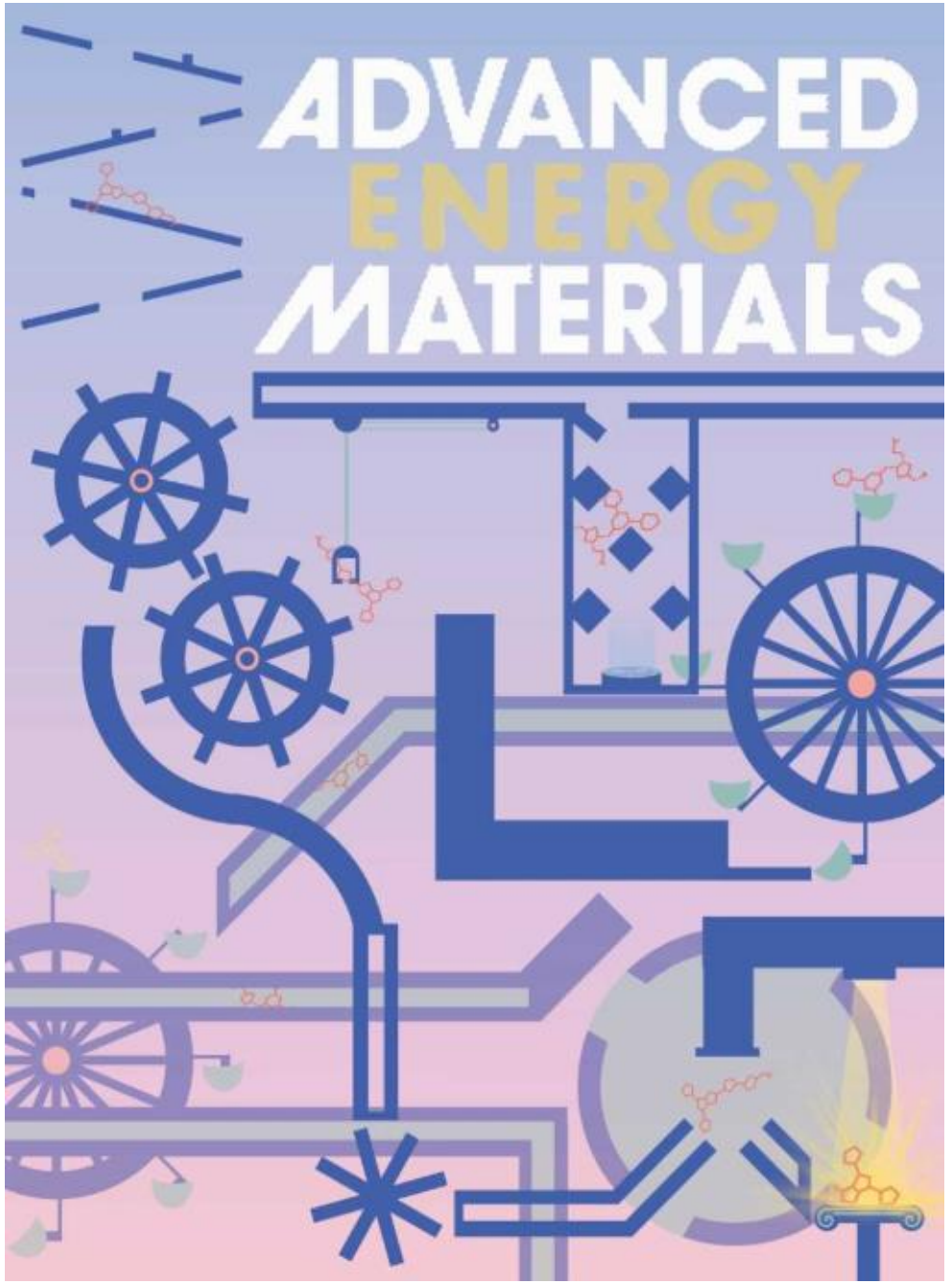
# Molecular Engineering

**of Functional Materials**

# Research Background with Central Facilities




STFC Rutherford Appleton Laboratory (& International Facilities)




Journal Impact Factor: 22


FULL PAPER

Dye-Sensitized Solar Cells

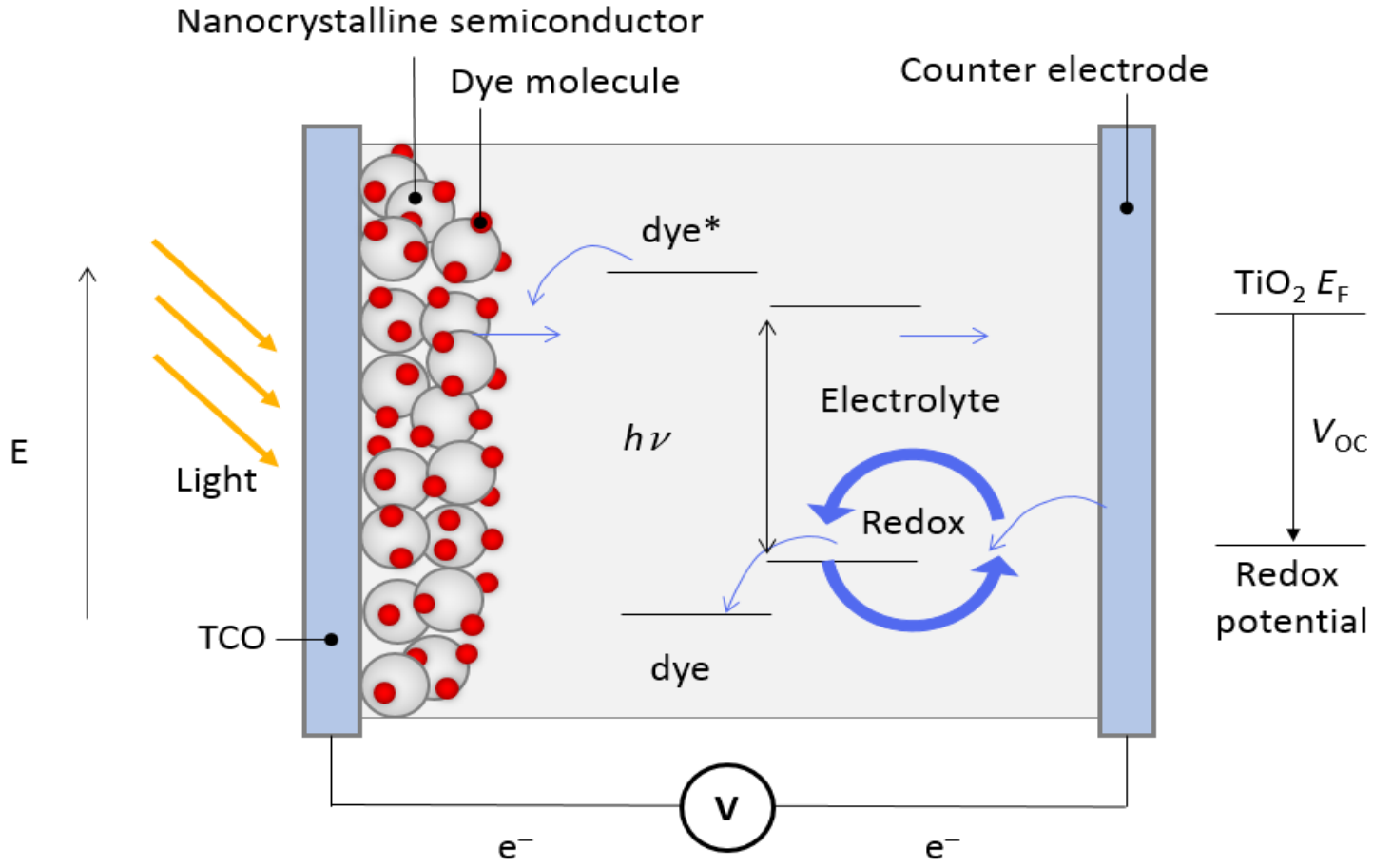
ADVANCED ENERGY MATERIALS

www.advenergymat.de

# Design-to-Device Approach Affords Panchromatic Co-Sensitized Solar Cells

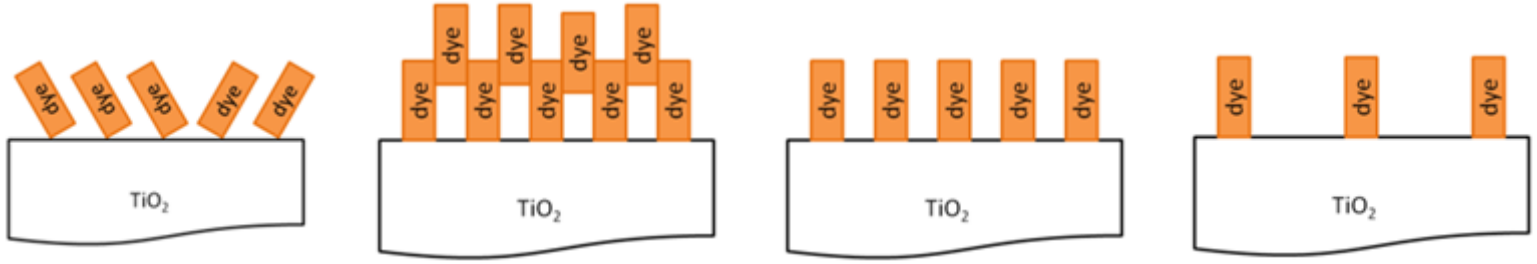
*Christopher B. Cooper, Edward J. Beard, Álvaro Vázquez-Mayagoitia, Liliana Stan, Gavin B. G. Stenning, Daniel W. Nye, Julian A. Vigil, Tina Tomar, Jingwen Jia, Govardhana B. Bodedla, Song Chen, Lucía Gallego, Santiago Franco, Antonio Carella, K. R. Justin Thomas, Song Xue, Xunjin Zhu, and Jacqueline M. Cole**

# Dye-sensitized solar cell

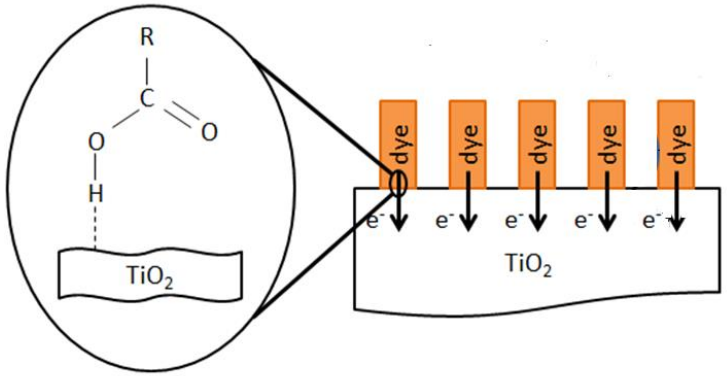



Graz Science Tower (Sep 17)

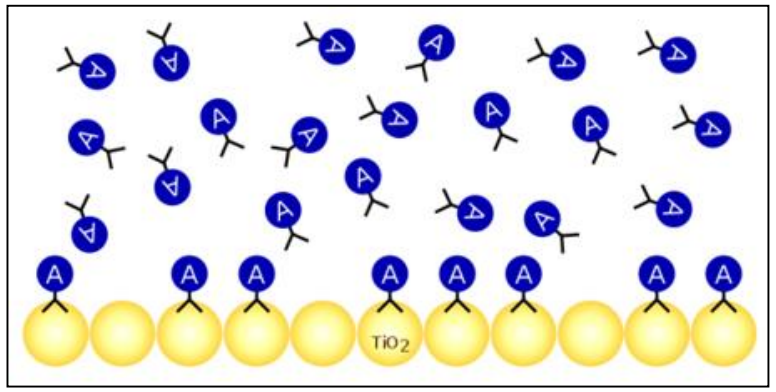
# Relating Molecular Structure to Device Function




**Dye orientation** **Dye aggregation** **Dye coverage** **Inter-dye spacing**

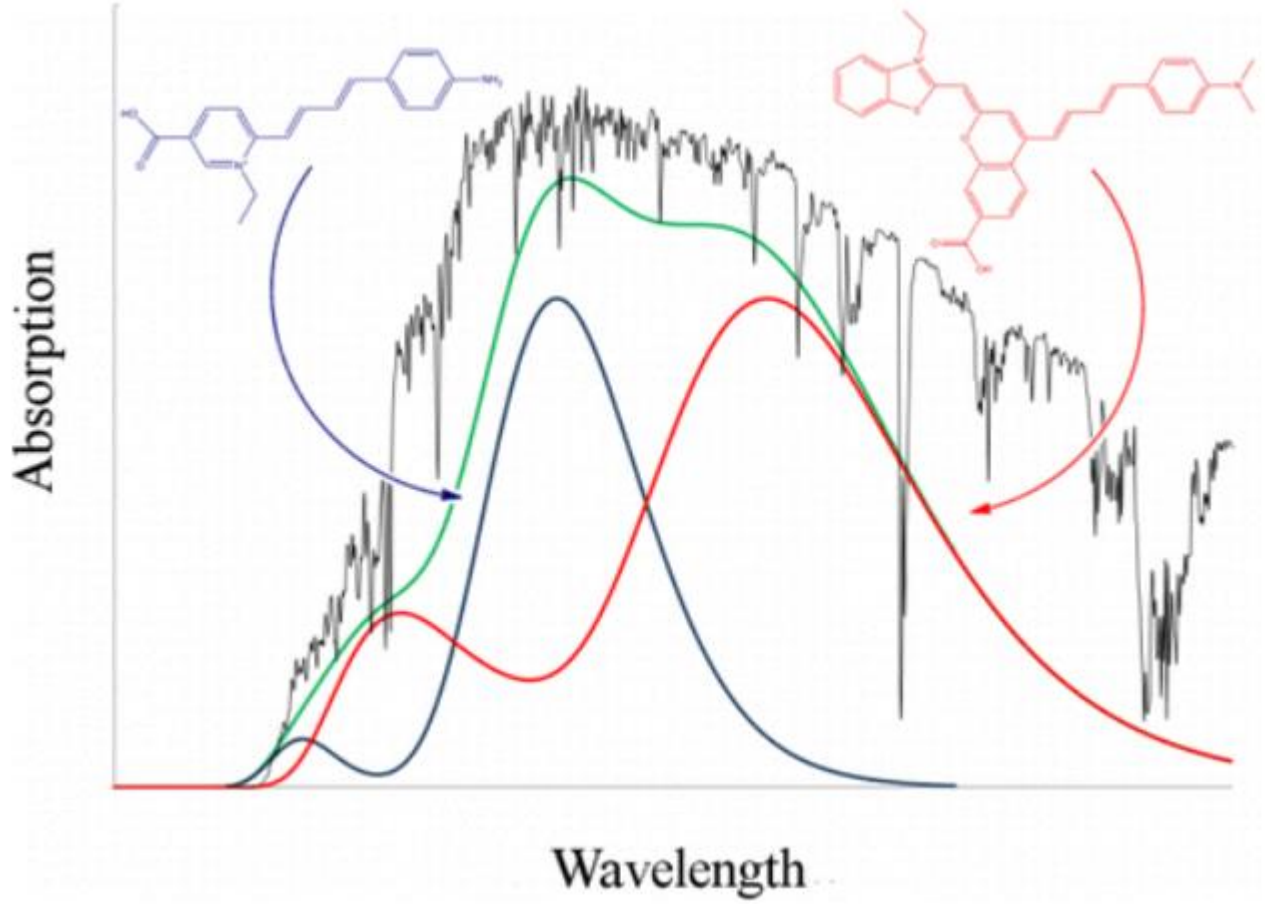


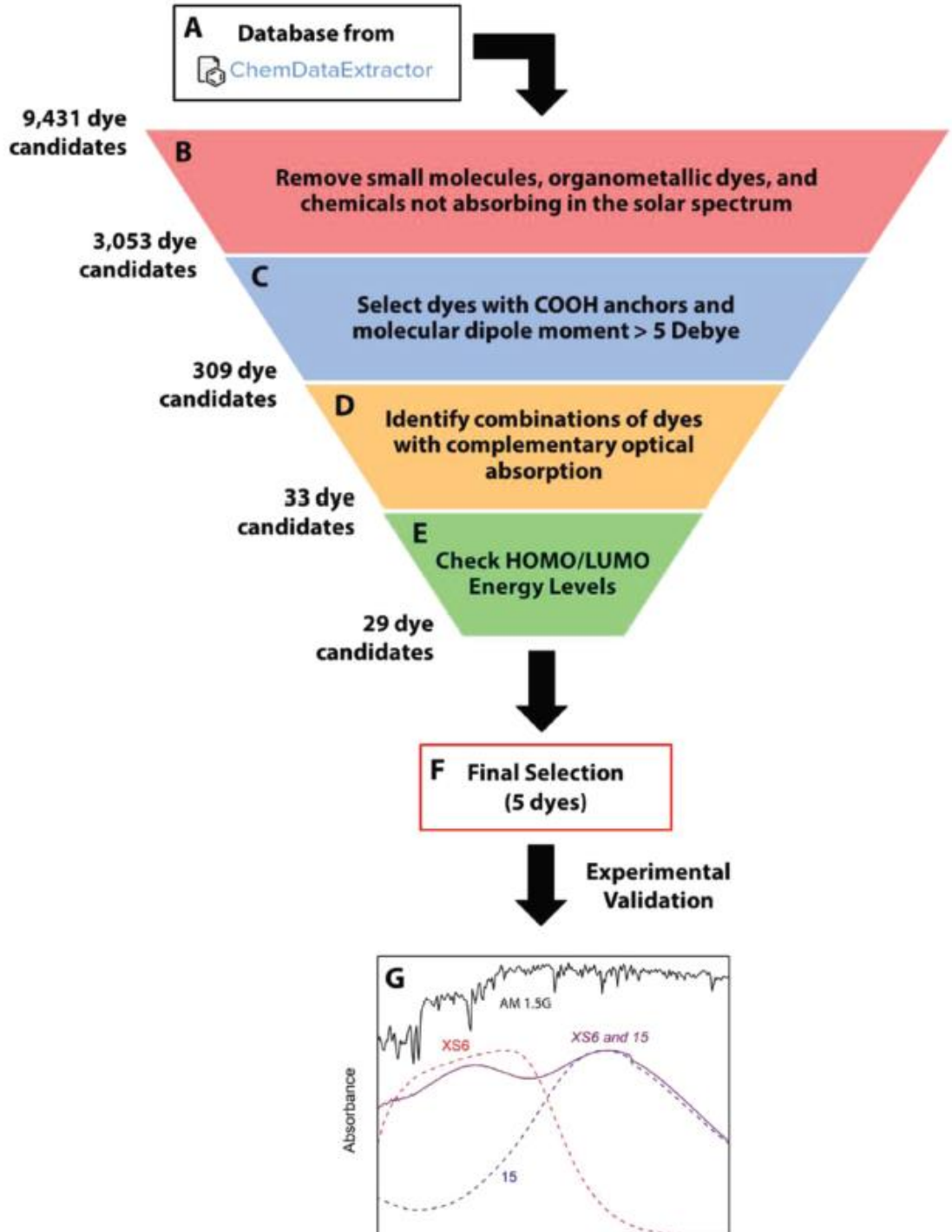

**Dye···$TiO_2$ binding**



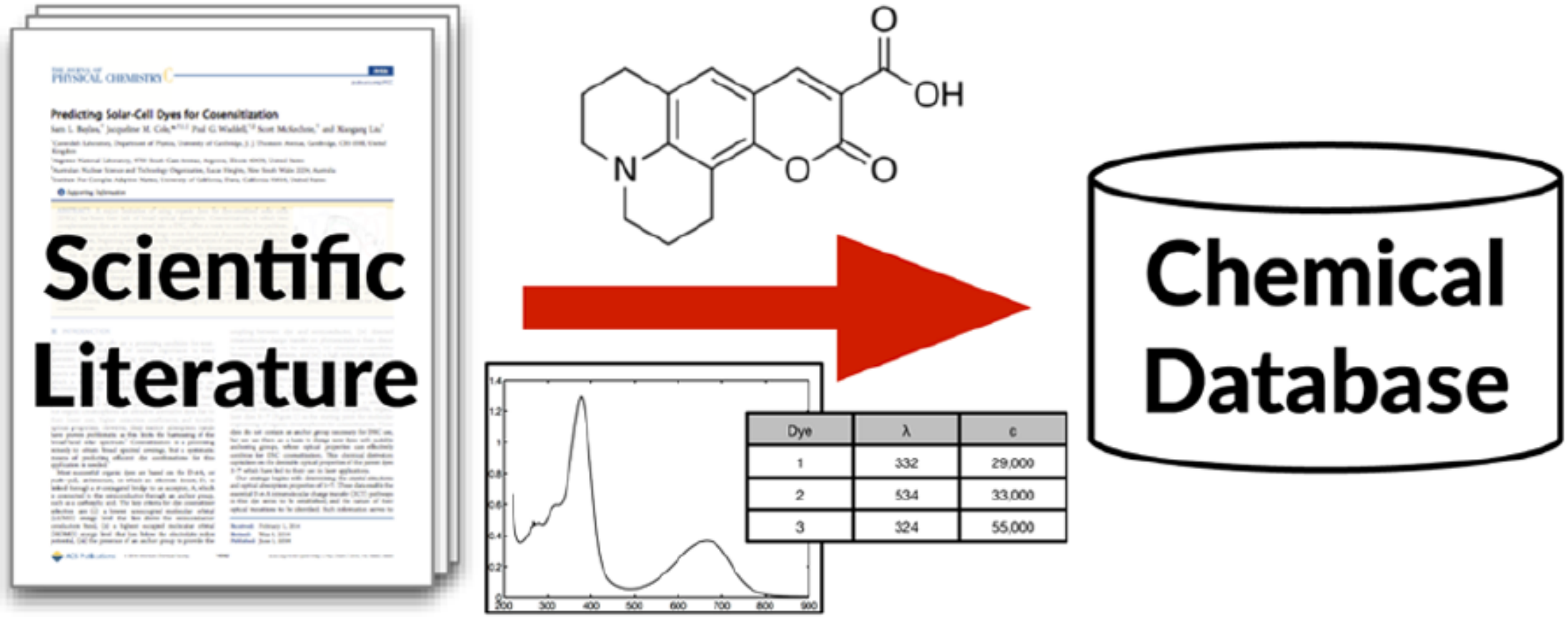

**Dynamic Processes**

# Co-sensitization



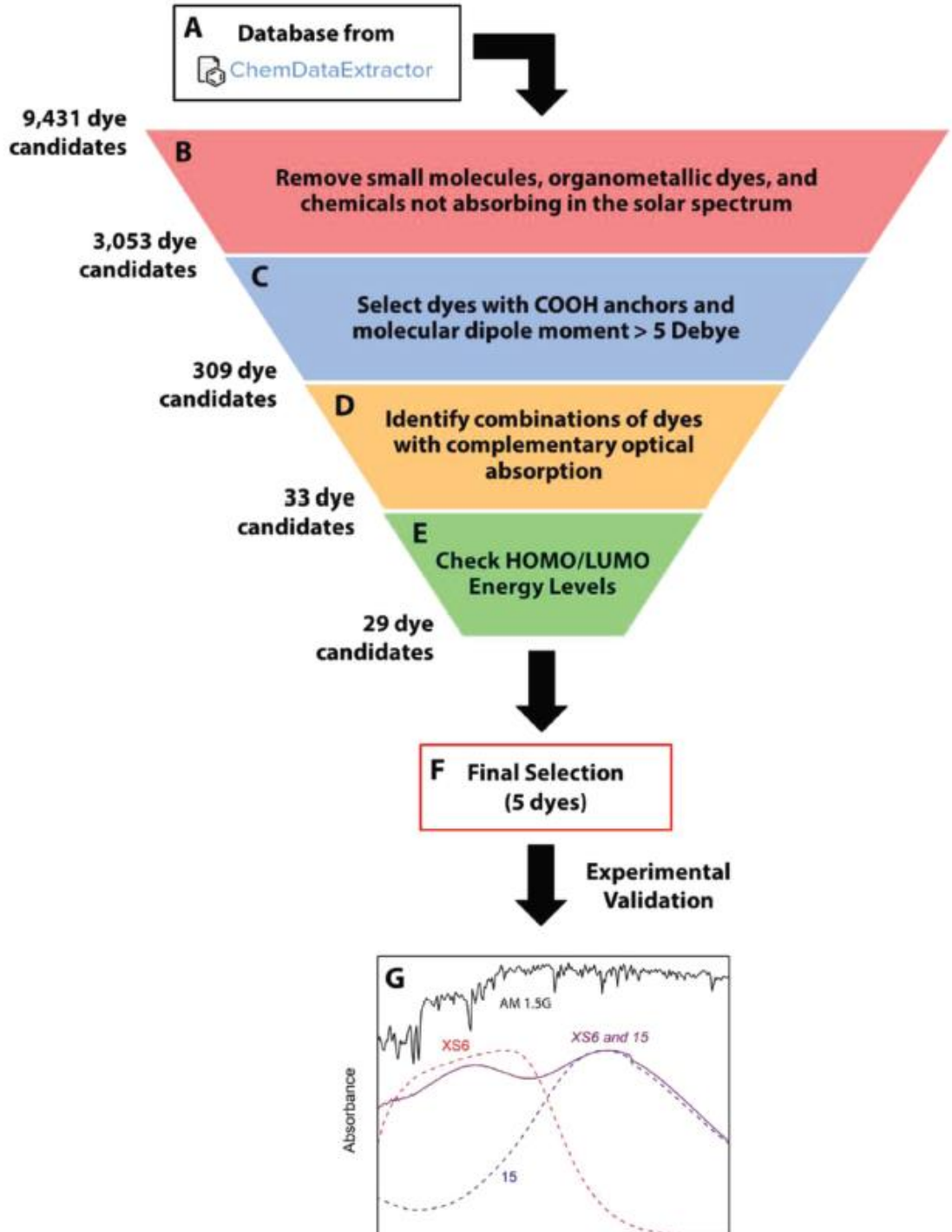

A
Database from
ChemDataExtractor
9,431 dye candidates
B
Remove small molecules, organometallic dyes, and chemicals not absorbing in the solar spectrum
3,053 dye candidates
C
Select dyes with COOH anchors and molecular dipole moment > 5 Debye
309 dye candidates
D
Identify combinations of dyes with complementary optical absorption
33 dye candidates
E
Check HOMO/LUMO Energy Levels
29 dye candidates
F
Final Selection (5 dyes)
Experimental Validation
G
AM 1.5G
XS6
XS6 and 15
15
Absorbance

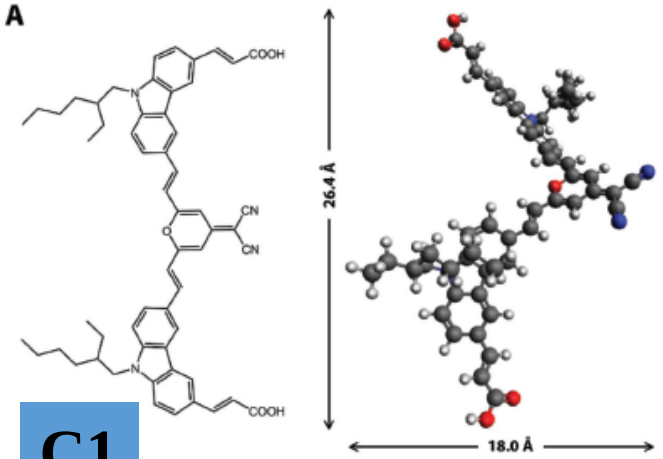
# ChemDataExtractor



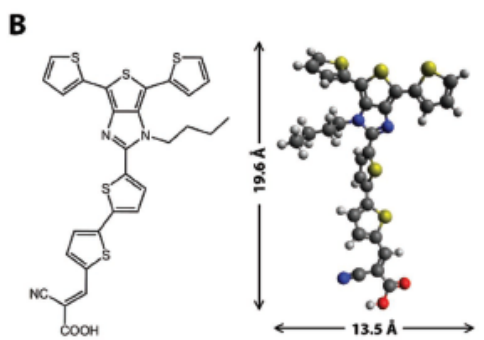

M. C. Swain, J. M. Cole *J. Chem. Inf. Model*. 56 (2016) 1894-1904

www.chemdataextractor.org

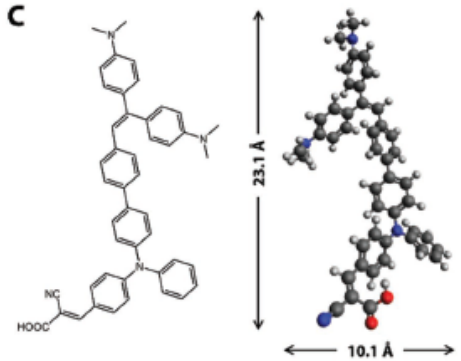

A
Database from
ChemDataExtractor
9,431 dye candidates
B
Remove small molecules, organometallic dyes, and chemicals not absorbing in the solar spectrum
3,053 dye candidates
C
Select dyes with COOH anchors and molecular dipole moment > 5 Debye
309 dye candidates
D
Identify combinations of dyes with complementary optical absorption
33 dye candidates
E
Check HOMO/LUMO Energy Levels
29 dye candidates
F
Final Selection (5 dyes)
Experimental Validation
G
AM 1.5G
XS6
XS6 and 15
15
Absorbance



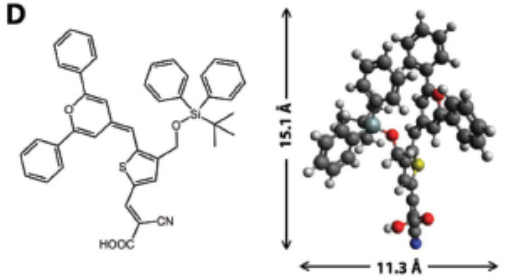

C1



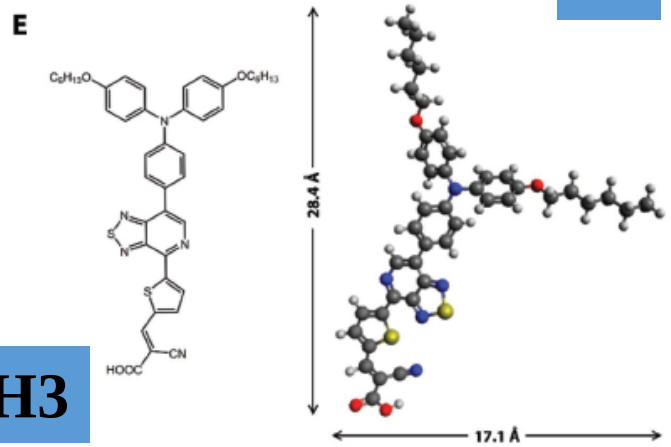

8c



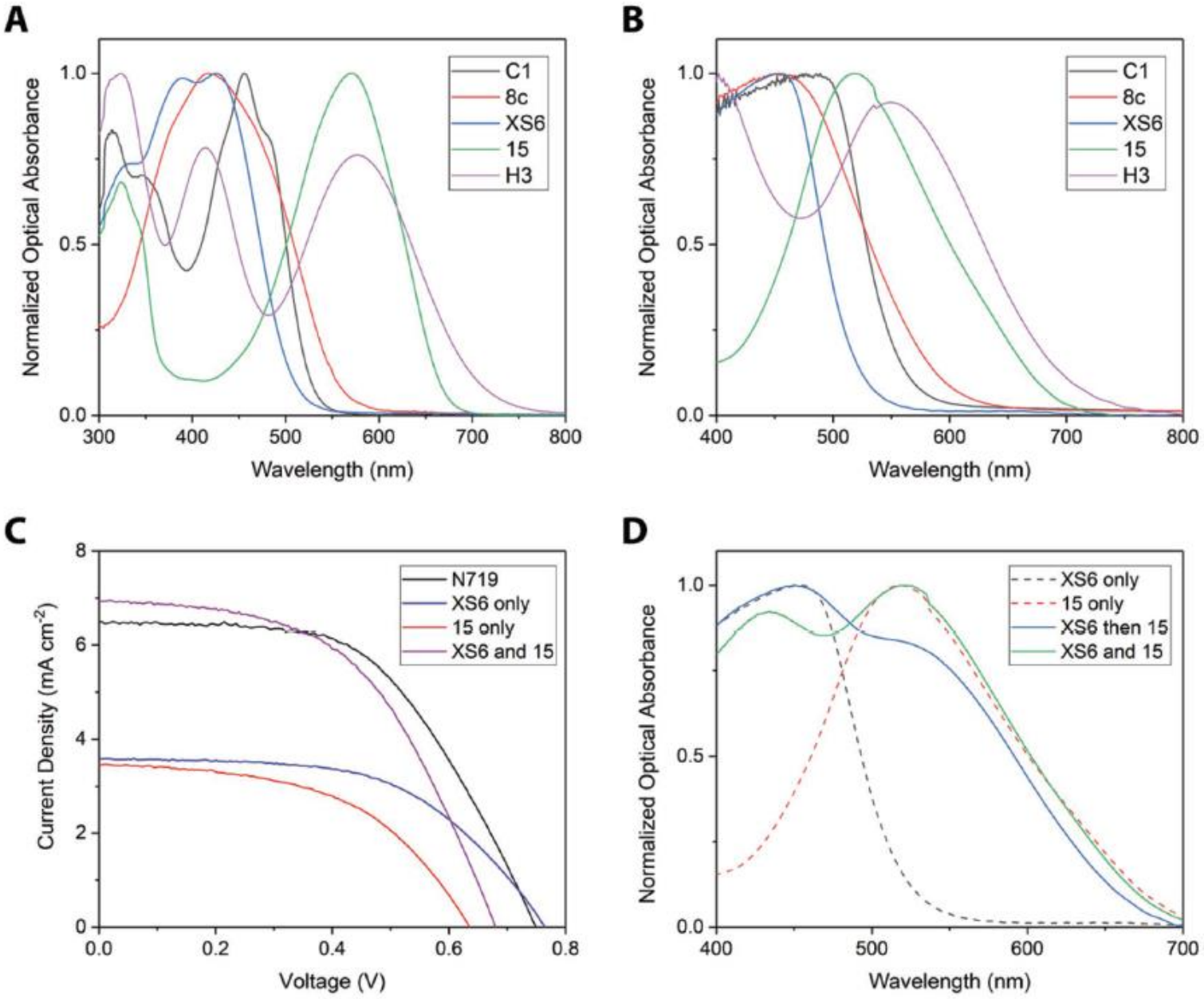

XS6




15



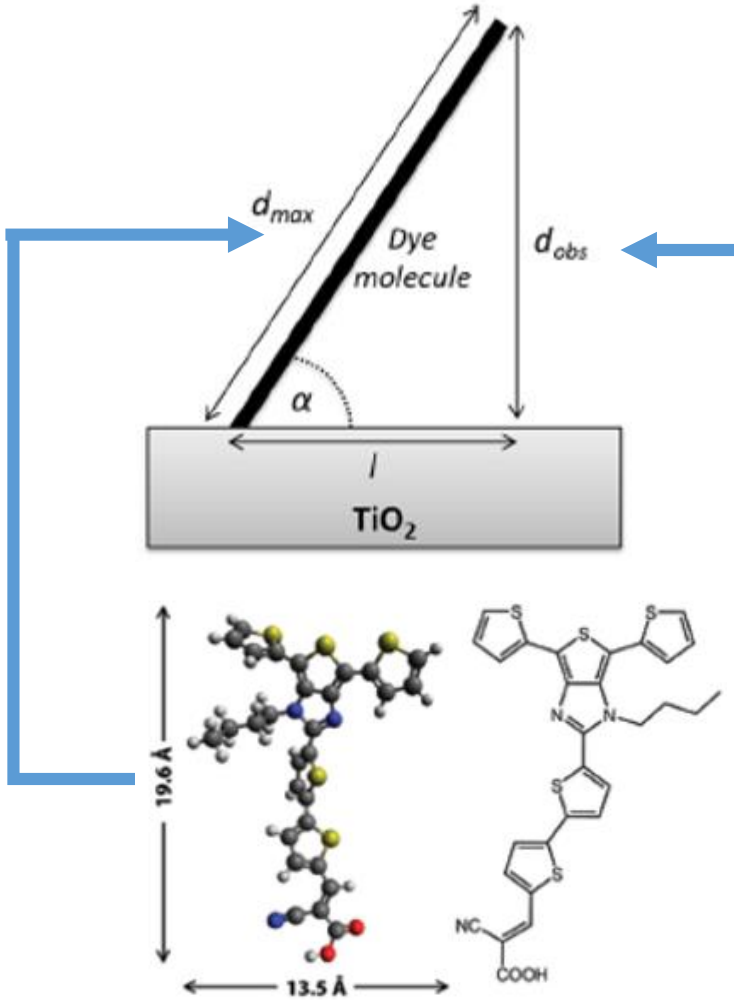

H3

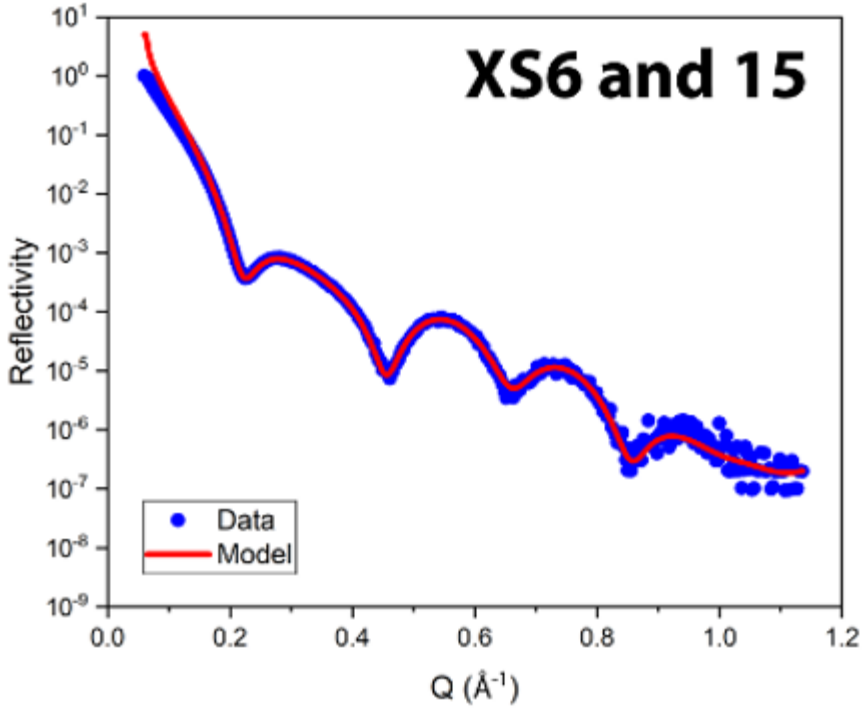



PV device output: XS6 67%; 15 51%; XS6/15 82%; XS6&15 92% of industry standard (N719)

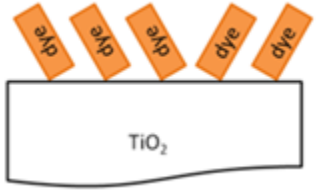
# Advanced Materials Characterization

# X-ray reflectometry



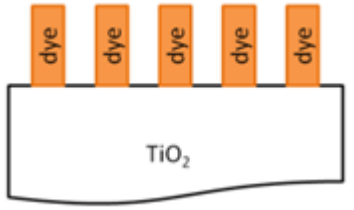



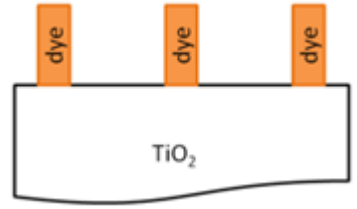

| Dye layer thickness [Å] | $SLD_{dye}$ [$\times 10^{-6}$ Å$^{-2}$] | Surface roughness [Å] |
|---|---|---|
| Surface coverage [%] | $SLD_{ideal} = \frac{r_e Z}{V}$ $x = \frac{SLD_{measured}}{SLD_{ideal}}$ | |



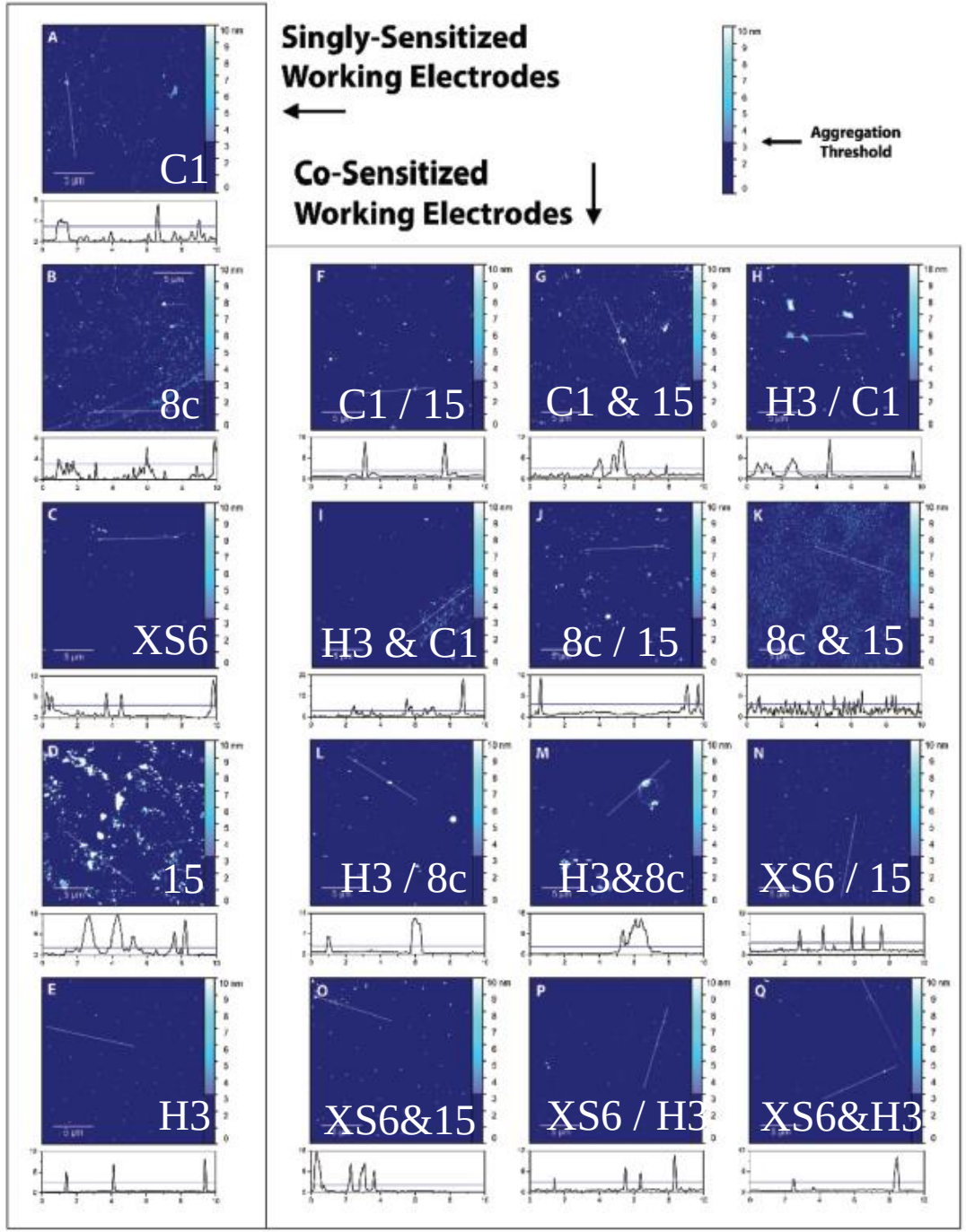

**Dye orientation**

| Sample name | XRR parameters | | | |
|---|---|---|---|---|
| | Dye layer thickness [Å] | $SLD_{dye}$ [$\times 10^{-6}$ Å$^{-2}$] | Surface roughness [Å] | Surface coverage [%] |
| Singly sensitized | | | | |
| C1 only | 43.5 ± 0.9 | 6.6 ± 0.5 | 5.6 ± 0.7 | 55 ± 4 |
| 8c only | 26.6 ± 0.9 | 5.1 ± 0.9 | 3.3 ± 0.8 | 39 ± 7 |
| XS6 only | 23.6 ± 0.5 | 8.7 ± 0.4 | 3.7 ± 0.5 | 73 ± 3 |
| H3 only | 27 ± 1 | 6.7 ± 0.5 | 3.7 ± 0.5 | 55 ± 4 |
| 15 only | 24.3 ± 0.3 | 7.8 ± 0.4 | 2.7 ± 0.3 | 62 ± 3 |
| Co-sensitized | | | | |
| *C1 then 15* | 33.7 ± 0.5 | 5.9 ± 0.7 | 3.1 ± 0.6 | 49 ± 6 |
| *C1 and 15* | 21.5 ± 0.8 | 6.3 ± 0.9 | 3.8 ± 0.7 | 52 ± 7 |
| *H3 then C1* | 42 ± 1 | 6.0 ± 0.6 | 5.2 ± 0.7 | 49 ± 5 |
| *C1 and H3* | 25.4 ± 0.4 | 8.5 ± 0.4 | 3.0 ± 0.5 | 69 ± 3 |
| *8c then 15* | 30.9 ± 0.4 | 6.9 ± 0.4 | 3.9 ± 0.6 | 54 ± 3 |
| *8c and 15* | 31 ± 2 | 5.7 ± 0.5 | 7 ± 2 | 45 ± 4 |
| *H3 then 8c* | 37.2 ± 0.2 | 9.0 ± 0.7 | 2.9 ± 0.4 | 70 ± 5 |
| *8c and H3* | 27.5 ± 0.4 | 8.0 ± 0.4 | 3.3 ± 0.6 | 63 ± 3 |
| ***XS6 then 15*** | **18.8 ± 0.3** | **8.7 ± 0.5** | **3.6 ± 0.4** | **72 ± 4** |
| ***XS6 and 15*** | **18.6 ± 0.3** | **8.8 ± 0.5** | **3.4 ± 0.4** | **73 ± 4** |
| *XS6 then H3* | 21.0 ± 0.3 | 9.6 ± 0.5 | 4.1 ± 0.4 | 79 ± 4 |
| *XS6 and H3* | 21.6 ± 0.6 | 8.7 ± 0.6 | 4.0 ± 0.5 | 71 ± 5 |

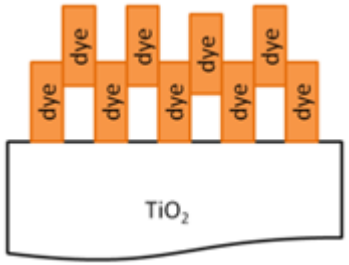


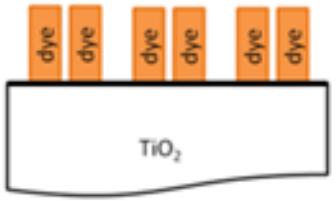




**Dye coverage**


Singly-Sensitized
Working Electrodes
Co-Sensitized
Working Electrodes
Aggregation
Threshold
A
C1
B
8c
C
XS6
D
15
E
H3
F
C1 / 15
G
C1 & 15
H
H3 / C1
I
H3 & C1
J
8c / 15
K
8c & 15
L
H3 / 8c
M
H3&8c
N
XS6 / 15
O
XS6&15
P
XS6 / H3
Q
XS6&H3

| Sample name | AFM parameters | | | |
|---|---|---|---|---|
| | Mean height [nm] | Max height [nm] | Aggregate coverage [%] | Number of aggregates [$\mu m^{-2}$] |
| Singly sensitized working electrodes | | | | |
| C1 only | 5 ± 1 | 7 ± 2 | 3 ± 6 | 2 ± 3 |
| 8c only | 5 ± 1 | 6 ± 2 | 3 ± 2 | 3 ± 2 |
| XS6 only | 4.9 ± 0.4 | 6.0 ± 0.7 | 1.0 ± 0.1 | 0.3 ± 0.2 |
| H3 only | 9 ± 1 | 15 ± 3 | 0.3 ± 0.1 | 0.18 ± 0.05 |
| 15 only | 8 ± 2 | 15 ± 3 | 7 ± 2 | 1.1 ± 0.4 |
| Co-sensitized working electrodes | | | | |
| *C1 then 15* | 6 ± 2 | 10 ± 3 | 1.3 ± 0.5 | 0.7 ± 0.2 |
| *C1 and 15* | 7 ± 2 | 12 ± 4 | 2.0 ± 0.5 | 0.9 ± 0.6 |
| *H3 then C1* | 8 ± 2 | 16 ± 4 | 3 ± 3 | 0.4 ± 0.2 |
| *C1 and H3* | 5 ± 1 | 8 ± 3 | 2 ± 1 | 2 ± 2 |
| *8c then 15* | 6 ± 1 | 9 ± 2 | 1.1 ± 0.2 | 0.7 ± 0.6 |
| *8c and 15* | 4.6 ± 0.3 | 5.8 ± 0.4 | 12 ± 9 | 16 ± 5 |
| *H3 then 8c* | 5.5 ± 0.7 | 8 ± 1 | 3 ± 2 | 1 ± 1 |
| *8c and H3* | 5.2 ± 0.7 | 7 ± 2 | 2 ± 2 | 1 ± 1 |
| ***XS6 then 15*** | **6 ± 1** | **8 ± 2** | **0.7 ± 0.3** | **0.8 ± 0.3** |
| ***XS6 and 15*** | **7.8 ± 0.7** | **11 ± 1** | **0.3 ± 0.1** | **0.24 ± 0.09** |
| *XS6 then H3* | 5.5 ± 0.7 | 7.6 ± 0.8 | 0.3 ± 0.1 | 0.25 ± 0.04 |
| *XS6 and H3* | 5.3 ± 0.8 | 7 ± 1 | 0.3 ± 0.1 | 0.2 ± 0.1 |




**Dye aggregation**

# Conclusions

Design-to-Device approach to materials discovery (Data Science, computation, experiments)

Database auto-generation developments (ChemDataExtractor) successful for data science

One pair of lead dye candidates yields PV output ~ industry standard

Advanced Materials Characterisation at STFC RAL rationalises PV output

Development of Sample Environment for World Unique Instrumentation and Experiments

Great team work – 18 authors on AEM paper!

National and International Facilities (big data sources as well as experimental resources)