UNIVERSITY OF CAMBRIDGE

Co-sensitization in Dye-Sensitized Solar Cells

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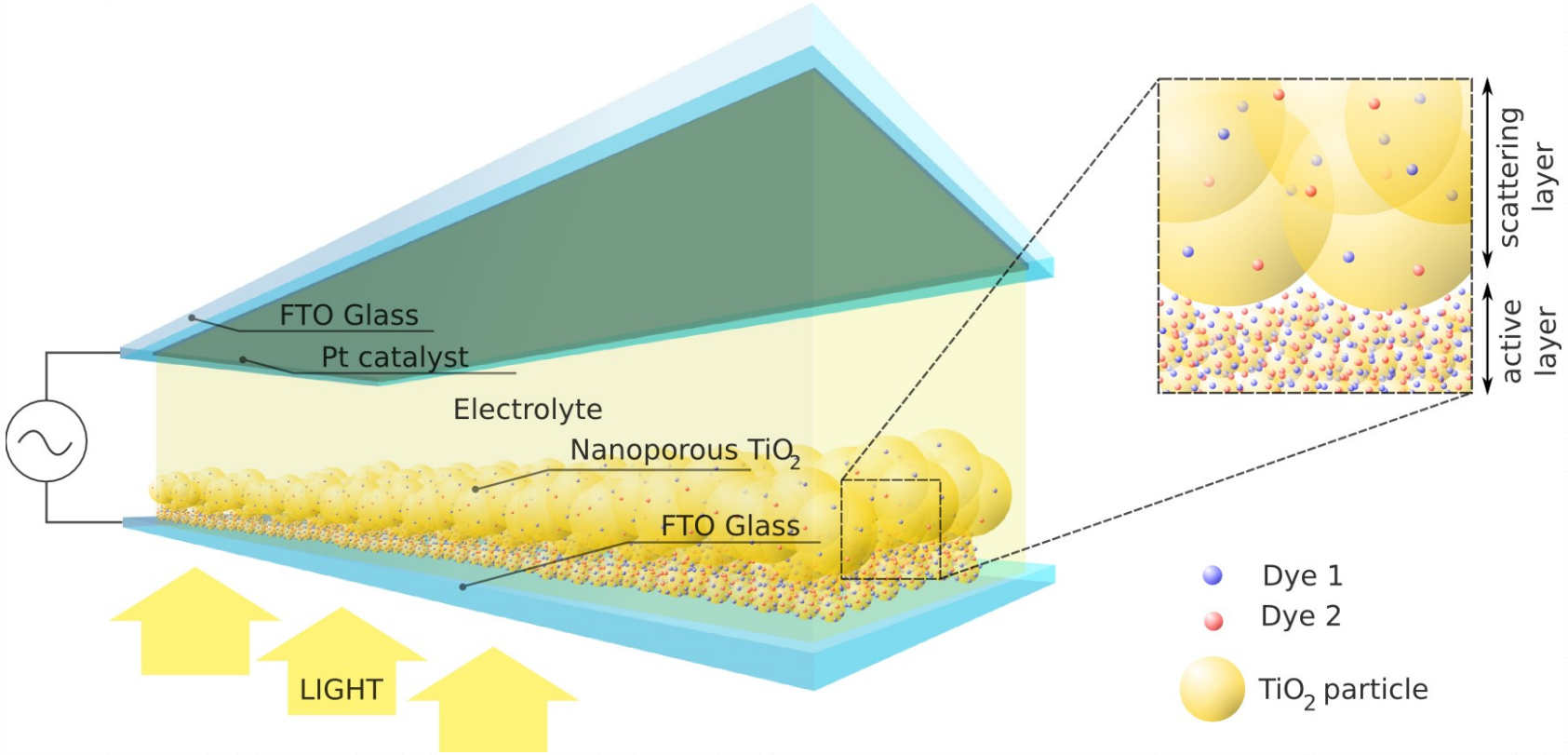
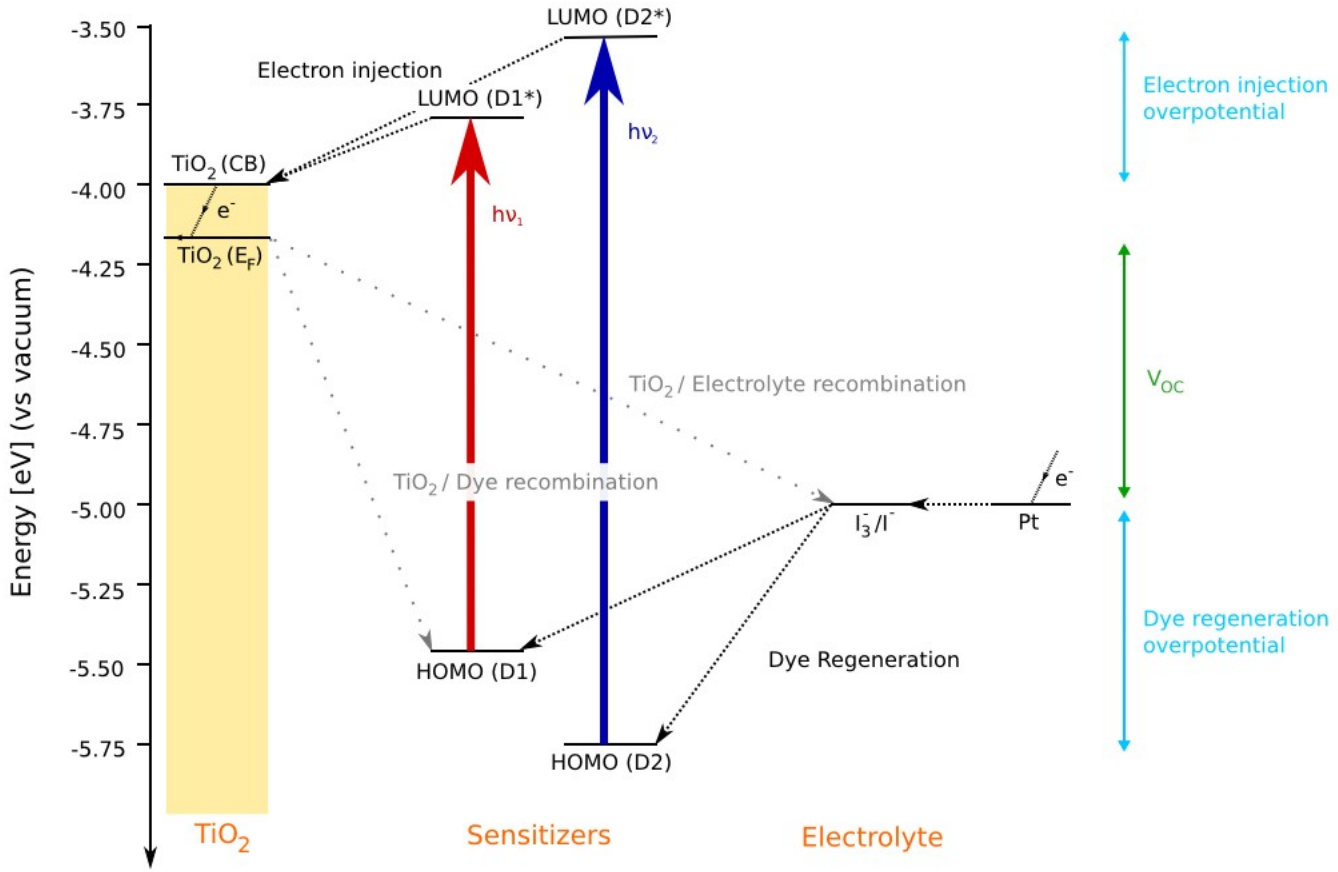
About me

- **University College London (2008-2011) – B.Sc Physics**
- **Institut Laue Langevin (2011) – Intern**
  Magnetic structure of MnPS3 from neutron diffraction data
- **University College London (2012) – M.Sci Physics**
  Analysis of jet substructure from W and Z boson decays (LHC)
- **University of Cambridge (2012-hopefully soon) – Ph.D. Physics**
  Structure-property relationships of dye molecules for predictions of suitable dyes in Co-sensitized Dye-Sensitized Solar Cells

Dye-Sensitized Solar Cells

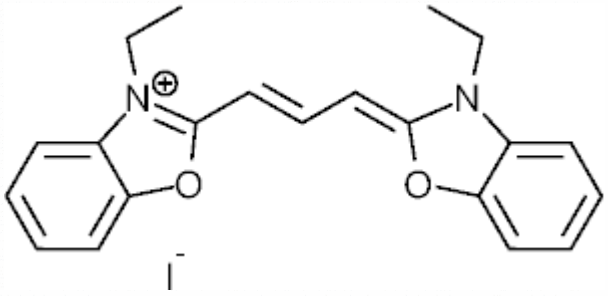


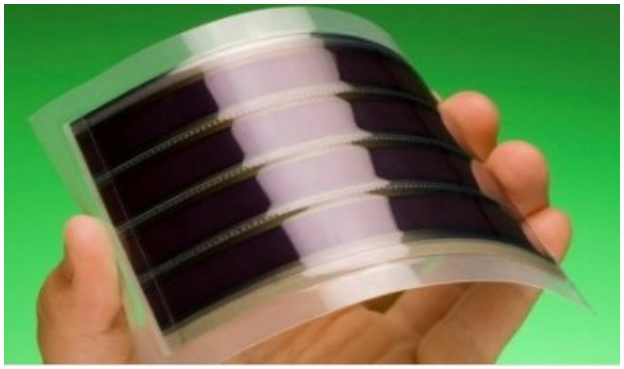
Dye-Sensitized Solar Cells



The experimental part...

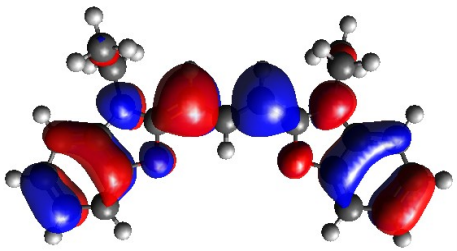
- **Measuring dye molecular opto-electronic properties:**
  - Single crystal X-ray diffraction
  - UV/visible spectroscopy
  - Cyclic voltammetry
  - Nuclear Magnetic Resonance
- **Dye-sensitized solar cell fabrication**

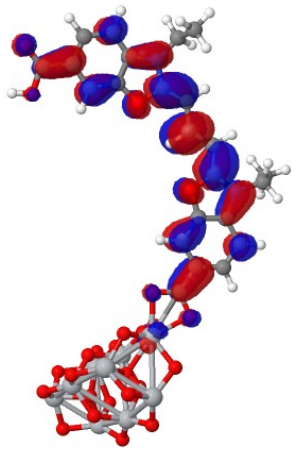


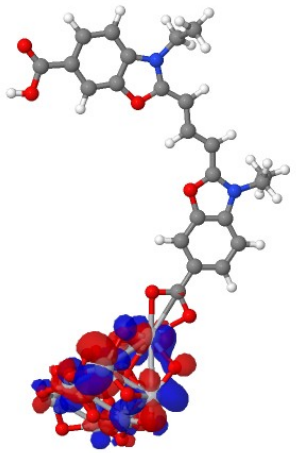


The computational part...

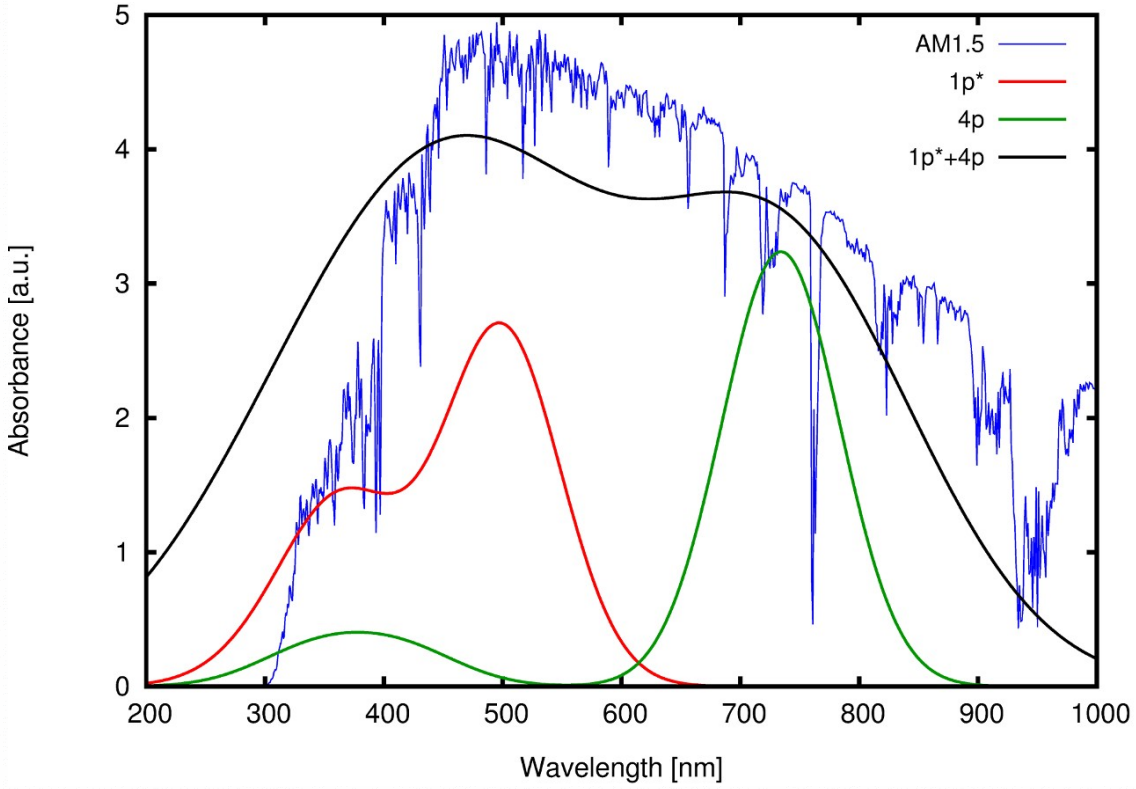
- **Modeling dye molecule structure and energies:**
  - Density Functional Theory
  - Time-Dependent Density Functional Theory
  - Coupled-clusters methods
  - Dye-TiO2 interface interaction
- **Molecular engineering new dyes**







Results


AM1.5
1p*
4p
1p*+4p
Absorbance [a.u.]
Wavelength [nm]
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1
2
3
4
5
200
300
400
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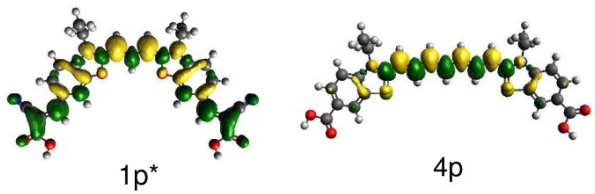
600
700
800
900
1000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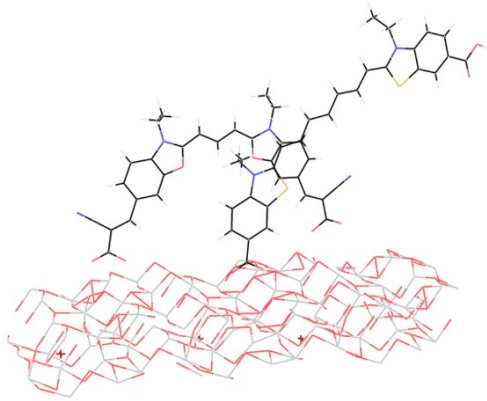

...and now the interesting part

Data mining with molecular design rules identifies new class of dyes for dye-sensitised solar cells†

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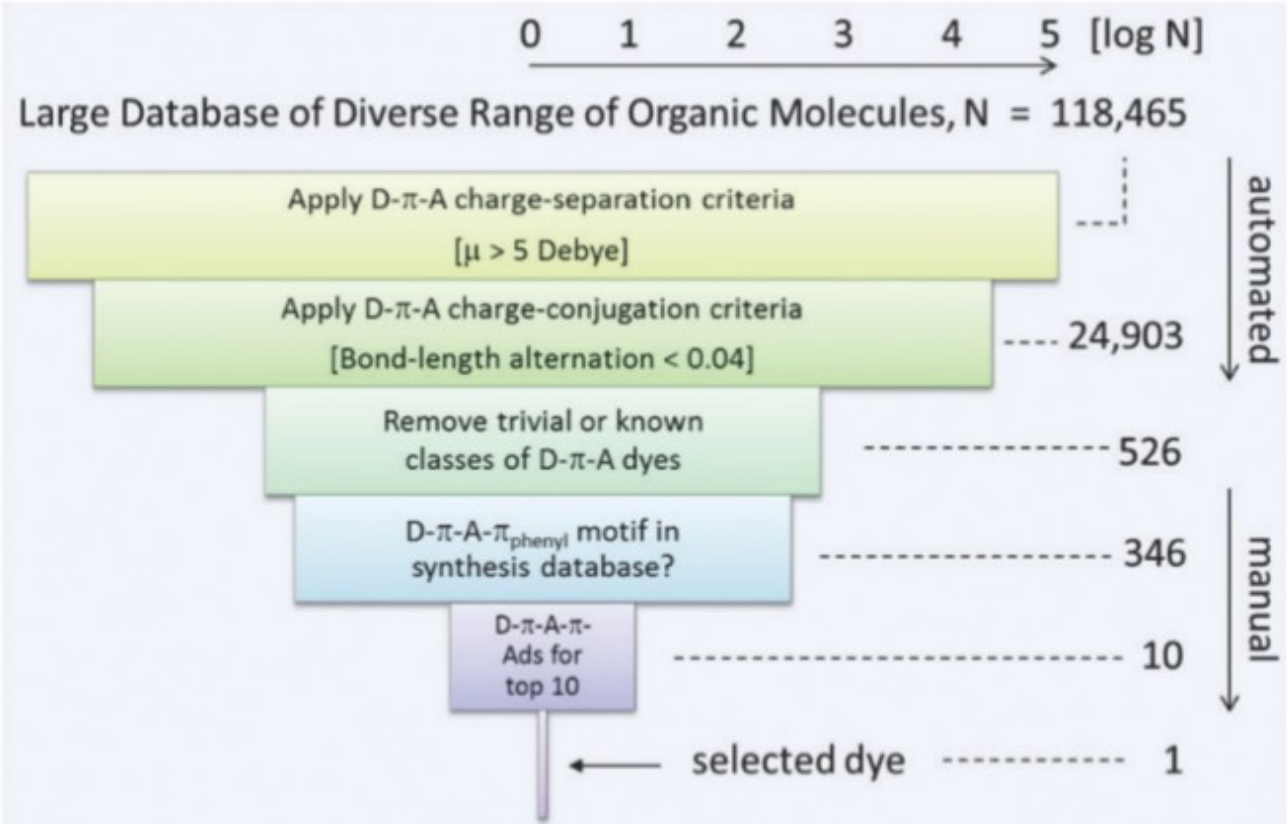
A major deficit in suitable dyes is stifling progress in the dye-sensitised solar cell (DSC) industry. Materials discovery strategies have afforded numerous new dyes; yet, corresponding solution-based DSC device performance has little improved upon 11% efficiency, achieved using the N719 dye over two decades ago. Research on these dyes has nevertheless revealed relationships between the molecular structure of dyes and their associated DSC efficiency. Here, such structure–property relationships have been codified in the form of molecular dye design rules, which have been judiciously sequenced in an algorithm to enable large-scale data mining of dye structures with optimal DSC performance. This affords, for the first time, a DSC-specific dye-discovery strategy that predicts new classes of dyes from surveying a representative set of chemical space. A lead material from these predictions is experimentally validated, showing DSC efficiency that is comparable to many well-known organic dyes. This demonstrates the power of this approach.

photovoltaic technology. Although less efficient than silicon-based solar cells, DSCs are far more cost-effective to the extent that their price-to-performance ratio achieves 'grid-parity' status, *i.e.* they are competitive with fossil-fuel energy production.

DSCs arose from the pioneering work of O'Regan and Grätzel[1] and are based upon a chemical photosynthetic redox process. The molecular dye is a particularly critical component of a DSC since it is responsible for both the light-harvesting of energy from the sun, and electron injection that initiates the chemical redox reaction of the solar cell. Consequently, there have been extensive efforts to discover new materials that outperform the ruthenium-based dye, N719 (10–10.4% solar-cell efficiency[2]), which remained the world's most efficient dye for DSCs for over 20 years. A major breakthrough finally came in 2011 with the report[3] of a zinc porphyrin-based dye which broke this world record, affording 12.3% under 1 sun illumination, when coupled with a cobalt-based electrolyte in a Grätzel cell. Last year, a solid-state DSC employing a lead-iodide based pigment surpassed

...and now the interesting part



Questions?

Thanks for listening!

Questions/comments?