

In-Licensing Opportunity – Novel characteristics to identify appropriate electron acceptors for organic photovoltaics

Prof Alessandro Troisi and his team at The University of Warwick have proven that a novel design rule applied is required to identify alternative organic acceptors to replace fullerene derivatives. Advantages include a proven design rule to develop cost-effective and more efficient organic solar cells.

BACKGROUND

Organic solar cells are among the most promising alternatives to traditional solar cells and offer the potential of low manufacturing, maintenance and installation cost.¹

A key challenge in organic solar cell development is finding an alternative electron acceptor material that can replace fullerene derivatives in these devices. Fullerene derivatives are used in the highest efficiency organic solar cells but they are not ideal because they do not absorb light, they are unlikely to become a low cost material and they pose further constraints (energy level alignment, miscibility) on the remaining components of the solar cell.^{2,3}

Replacing fullerene derivatives with alternative electron acceptors is therefore occupying a large number of research groups although the results have been until recently disappointing. Moreover, there seems to be no design rule that can help the development of new acceptors, let alone any proof that any such design rule does work.

INVENTION

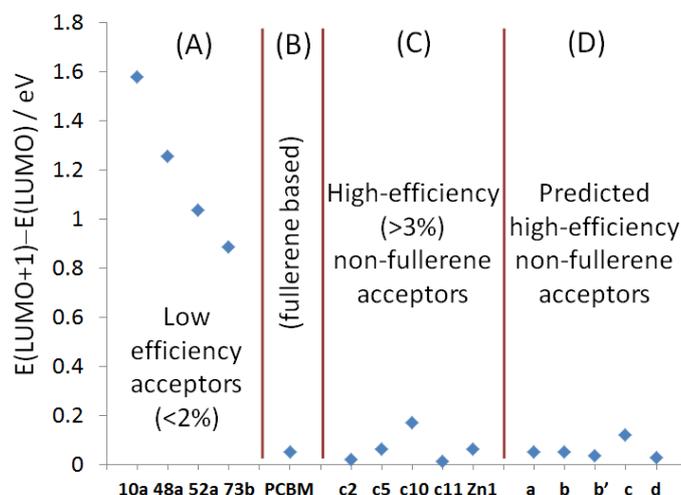
The Warwick team has developed and proven a design rule for the construction of a large family of suitable electron acceptor materials that can replace fullerene derivatives in organic photovoltaic devices. Such a rule lends itself to assisting in the design and syntheses of suitable electron acceptors or screening large sets of known molecules.

On the basis of electron transfer theory we have found that the presence of a virtual energy level (LUMO+1) close in energy to the LUMO level of the acceptor enhances the exciton dissociation into free charges by more than one order of magnitude.⁴ There is now robust experimental evidence that such a rule is highly relevant in designing any high efficiency electron acceptor.

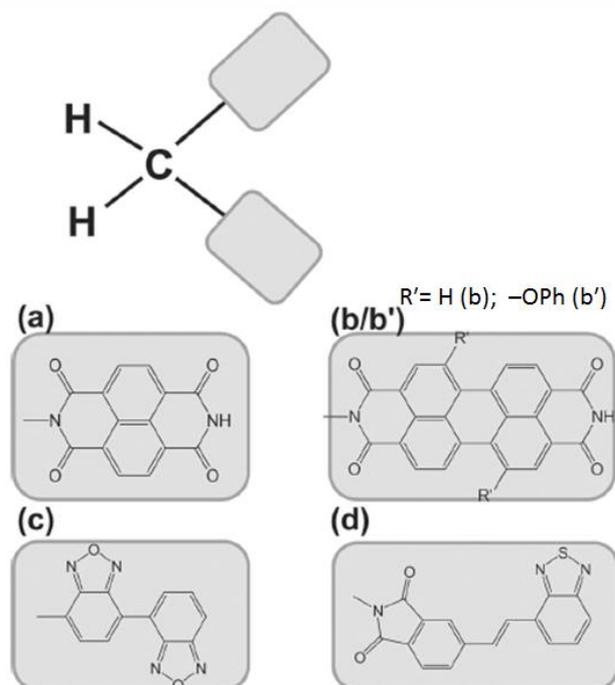
The diagram below reports the energy difference between computed LUMO+1 and LUMO energy levels for the following:

- (A) a set of acceptors from an old review,² all with power conversion efficiency (PCE) not exceeding 2%.
- (B) PCBM (the most used fullerene-based acceptor) whose typical efficiency is 8%.
- (C) the **complete** set of acceptors from a recent review³ with efficiency higher than 3% and another Zn-containing acceptor⁵ with efficiency 4%.
- (D) the predicted new acceptors proposed by the Warwick team and recently published⁴.

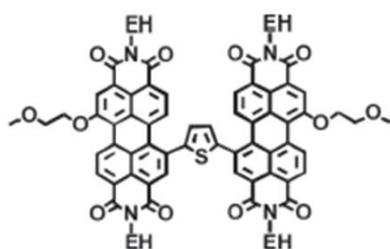
The labels in the horizontal axis refer to the compounds given in the corresponding reference. The diagram illustrates that a generic acceptor (group A) does not have low LUMO+1/LUMO gap. **All high-efficiency non-fullerene acceptors** in the diagram (group C) **appeared in literature after our original prediction**. Without known exceptions so far the highest efficiency acceptors satisfy the condition that the energy difference between LUMO+1 and LUMO is below 0.2 eV.



The property of having low LUMO+1/LUMO gap can be engineered as illustrated by the molecules in group (D) whose chemical structure is reproduced below.



One of the predicted new acceptor molecules (**b**) was based on a dimer of the PDI chromophore. After our original publication a related PDI dimer shown below (**c5** in the diagram of the LUMO/LUMO+1 levels), which turned out to be a record breaking molecule with 4% PCE, was reported in the literature.⁶



The adoption of such a design rule will immediately provide a significant competitive advantage to companies seeking to become leading manufacturers of organic electron acceptor compounds.

Our patent application covers the design rule and the broad classification of compounds that can be constructed using this rule.

BENEFITS OF TECHNOLOGY

- ❖ Novel and proven design rule to select organic acceptor compounds for organic solar cells
- ❖ Targeted synthesis based on structure activity relationship
- ❖ Low manufacturing, maintenance and installation cost of organic solar cells
- ❖ Use of a low cost material for the development of more efficient photovoltaics
- ❖ Replaces shortcomings of existing fullerene derivatives such as their inability to absorb light, they are relatively expensive and their poor energy level alignment and poor miscibility on the remaining components of the solar cell.

REFERENCES

1. Dou, L. et al, *Adv. Mater.*, 25, 6642, 2013
2. Sonar, P. et al, *Energy Environ. Sci.*, 4, 1558, 2011
3. Lin, Y and Zhan, X, *Mater. Horiz.*, 2014,1, 470-488
4. Liu, T and Troisi, A., *Adv. Mater.* 25, 1038, 2013.
5. Mao, Z., et al, *Adv. Mater.*, 26, 6290, 2014.
6. Zhang, X., et al, *Adv. Mater.*, 25: 5791–5797, 2013

TARGET PARTNERS

The technology is expected to be of interest to companies who are developing compounds for research and possibly large scale production in the area of organic electronics.

PATENT & PUBLICATION

'What Makes Fullerene Acceptors Special as Electron Acceptors in Organic Solar Cells and How to Replace them', Tao Liu and Alessandro Troisi, *Adv. Mater.* 25, 1038-1041, 2013.

'Organic Electron Acceptor Compounds. International Patent Application No. PCT/GB2013/051484. Priority date, 6th June 2012. Publication No. WO2013/182847. Publication date, 12th June 2013.

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Warwick Ventures Ltd is the commercial arm of the University of Warwick.