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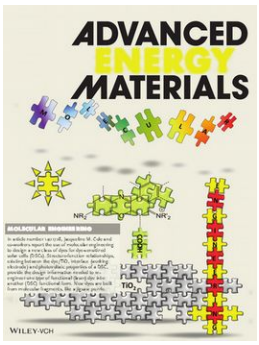
| 17 June 2015 | Jacqui Cole (Cambridge) | Molecular engineering of dyes for dye sensitized solar cells |


Dye-sensitized solar cells (DSCs) have unique attributes that afford them prospective applications as smart windows - windows in buildings that generate electricity from sunlight. This electricity will be fed into a local grid that will create sustainable buildings for future cities.




Materials discovery of new DSC dyes is one of the remaining bottlenecks to technological progress of smart windows. This talk shows we are attempting to overcome this materials bottleneck via two complementary routes to molecular design: (i) a 'top down' approach that uses large-scale data mining to identify brand new classes of DSC dyes [1]; (ii) a 'bottom up' approach that computationally transforms well-known non-DSC dyes into suitable DSC dyes [2,3].

The ‘top down’ approach involves large-scale data-mining to search for appropriate dye candidates [1]. Here, structure-property relationships for DSC dyes 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.

The ‘bottom up’ approach concerns case studies on families of well-known laser dyes that are transformed into functional DSC dyes using molecular engineering [2,3]. The underlying conceptual idea is to implement certain electronic structure changes in laser dyes, using molecular engineering, to make DSC-active dyes; while maintaining key property attributes of the laser dyes that are equally attractive to DSC applications. This requires a concerted experimental and computational approach; results predict new dye co-sensitizers for DSC applications.

**References**

[1] J. M. Cole, K. S. Low, H. Ozoe, P. Stathi, C. Kitamura, H. Kurata, P. Rudolf, T. Kawase, “Data Mining with Molecular Design Rules Identifies New Class of Dyes for Dye-Sensitised Solar Cells” *Phys. Chem. Chem. Phys*. 48 (2014) 26684-90 (selected for a cover in 28th Dec issue).

[2] S. L. Bayliss, J. M. Cole, P. G. Waddell, S. McKechnie, X. Liu, “Predicting solar-cell dyes for co-sensitization”, *J. Phys. Chem. C* 118 (2014) 14082–14090

[3] F. A. Y. N. Schroeder, J. M. Cole, P. G. Waddell, S. McKechnie, “Transforming benzophenoxazine laser dyes into chromophores for dye-sensitized solar cells: a molecular engineering approach”, *Advanced Energy Materials* (2015) 5 DOI: 10.1002/aenm.201401728 (frontispiece for 6th May issue: http://onlinelibrary.wiley.com/doi/10.1002/aenm.201570047/epdf)