Designing New Classes of Dyes for Dye-Sensitized Solar Cells: A Molecular Engineering Approach

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Abstract:
A major deficit in suitable dyes is stifling progress in the dye-sensitized 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. Two molecular engineering approaches are presented in this talk, which illustrate how one can exploit structure-property relationships to design new DSC dyes.

A ‘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. This demonstrates the power of this approach; and with further development of this systems-approach, the materials discovery of higher-performing materials is anticipated.

A ‘bottom up’ approach concerns case studies on families of well-known laser dyes that are transformed into functional DSC dyes using molecular engineering [2]. 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 parent laser dyes that are equally attractive to DSC applications. This requires a concerted experimental and computational approach, interleaving results from single crystal X-ray diffraction, UV-vis absorption spectroscopy, cyclic voltammetry, density functional theory, and time-dependent density functional theory. A comparison of the frontier molecular orbital energy levels with the conduction-band edge of the classic TiO2 DSC photoanode and the redox potential of a DSC electrolyte, allows the prediction of these re-functionalized parent laser dyes as dye co-sensitizers for DSC applications.

References

Wednesday, October 1, 2014
3:00 PM
Boggs 600

Within the “Women Leaders in Physics and Engineering” series, an informal coffee talk will be held immediately after the colloquium at 4pm in Stanley Thomas 201. At this meeting students will have the opportunity to ask the guest speaker about her career and her experience as a woman scientist. This event is intended primarily for women however, men who are interested in gender issues are also welcome. Undergraduate students, graduate students, postdocs, and faculty from all fields of science are invited to attend.