

Using the tools of complexity science to optimize solar cells

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Dye sensitized solar cells are a new type of solar cell that we have investigated from the theoretical point of view in the past few years. While we have a reasonable understanding of the basic principles of operation of these devices in practice nobody has any idea of how they should be improved. The system is complex, in the true sense of the word, and it is not possible to focus on the optimization of a single parameter.

One of the ingredients of a dye solar cell is the dye, i.e. a molecule that absorb light and is attached to an inorganic semiconductor, often titania. Many scientists are trying to design dyes that lead to the best possible efficient solar cell. Large tables exist of the efficiency of solar cells which different dyes but there seems not be an obvious correlation between efficiency and structure.

We have implemented an automatic procedure to compute the electronic structure properties of a large number of experimentally tested dyes and, for each of them, a large number of parameters (e.g. dipole moment, the molecular volume) that may be important in modulating their efficiency in a solar cell. In other words, we have a database with a list of computed properties and an experimental efficiency for many dyes.

These are the research questions:

- Is there any computed property (or function of the computed property) that is a good predictor of the efficiency of the dye?
- Is it possible to use the database to predict the efficiency of a new dye for which the same property can be computed? The time to compute these properties is orders of magnitude shorter than the time to make the molecule and perform the measurement.
- It is possible, alternatively, to conclude that there is no correlation in the data and therefore there is no hope to predict the performance of a dye from the known performances of other dyes?

This problem is analogous to the determination of structure property relationship of drugs, when the activity of many drugs is correlated with some physical property of the molecule and this correlation is used to determine the activity of a new drug.

This problem is about data analysis (all the available data are generated by us). The approach has never been followed in the past and it is potentially very innovative in the field of material science discovery. We have already plan to expand our database and so it will be possible to continue this type of analysis in a PhD project joint between an academics in statistics and myself in chemistry.

Further readings:

http://en.wikipedia.org/wiki/Dye-sensitized_solar_cell

http://en.wikipedia.org/wiki/Quantitative_structure%E2%80%93activity_relationship