Design and Discovery of Optimal Molecular Scale Solar Antennas

A Computational Method for Property Prediction

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Problem Description

- Molecular scale solar antennas are multi-component complex materials
- Due to the large number of variable components (structural features, etc.) there is a large search space of potential solar antennas.
- Synthesis and testing of materials is expensive, so testing all possible molecules is unreasonable.

Project Goals

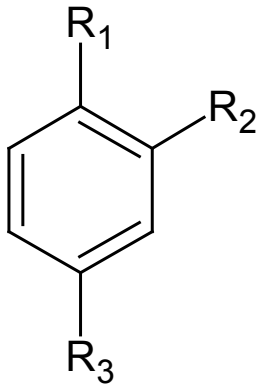
- Decrease the amount of synthesis and testing needed to find molecules with desired properties.
- Develop a property estimation method which uses a limited amount of laboratory data to predict the properties of untested molecules.

High Dimensional Model Representation

- If there are N independent variables describing a molecule from a certain library, a physical property of that molecule can be given as:

$$\text{Property} = F(x_1, x_2, \ldots x_N)$$

- Independent variables may be functional group substituent sites such as in a library of trisubstituted benzenes.



$F(R_1, R_2, R_3)$ can represent properties in this library

- This high dimensional function can be decomposed into a sum of lower order functions:

$$f_0 + \sum_{i=1}^{N} f_i(x_i) + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} f_{ij}(x_i, x_j) + \dots$$

- Each component function represents the contribution of one or several independent variables to the property value.

Genyuan Li, Carey Rosenthal, and Herschel Rabitz. High dimensional model representation. J. Phys. Chem. A, 105(33):7765,2001.

The Component Functions

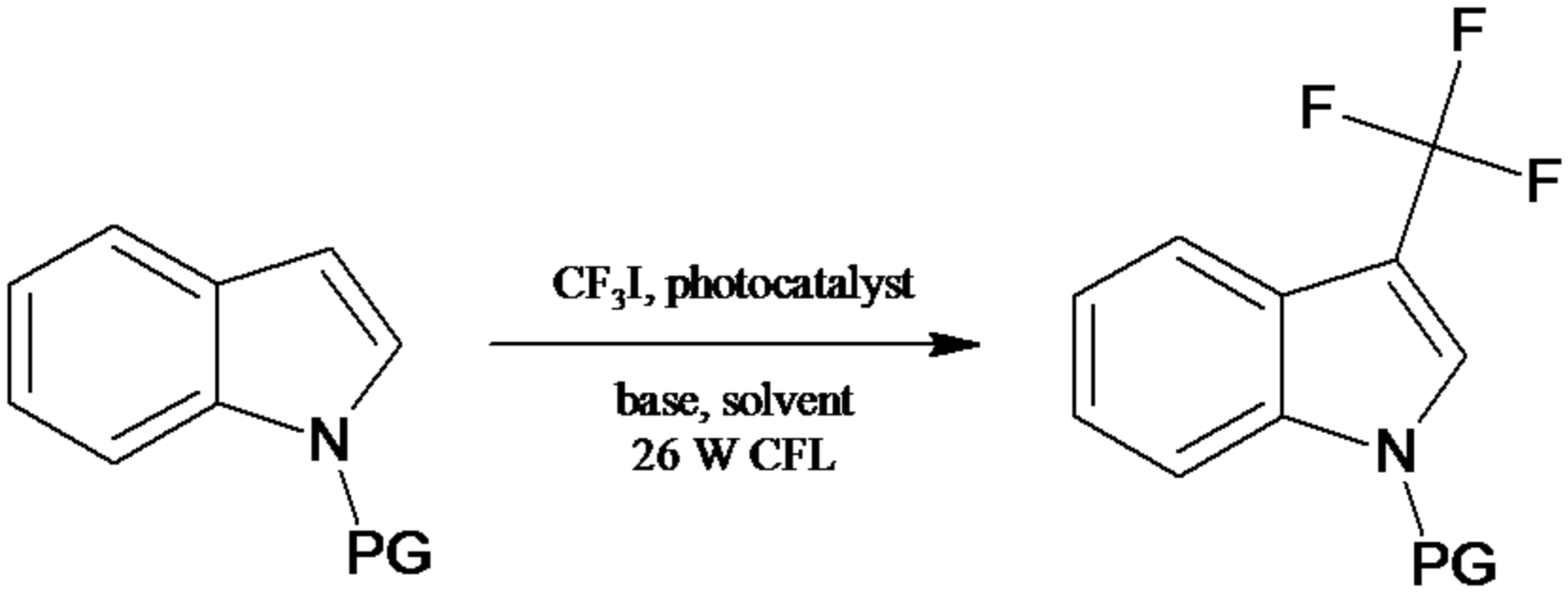
- f_0 if the base contribution to property value.
- $f_i(x_i)$ is the contribution of x_i acting alone
- $f_{ij}(x_i, x_j)$ is the contribution of x_i and x_j acting jointly.

- In other physical applications, joint contributions of many independent variables become insignificant compared to the individual contributions of those same variables so higher order decomposition terms can be ignored.

  Genyuan Li, Sheng-Wei Wang, and Herschel Rabitz. Practical Approaches to Construct RS-HDMR Component Functions. J. Phys. Chem. A, 106:8721,2002.

- It is much easier to determine several lower order component functions than the original high-dimensional property function.

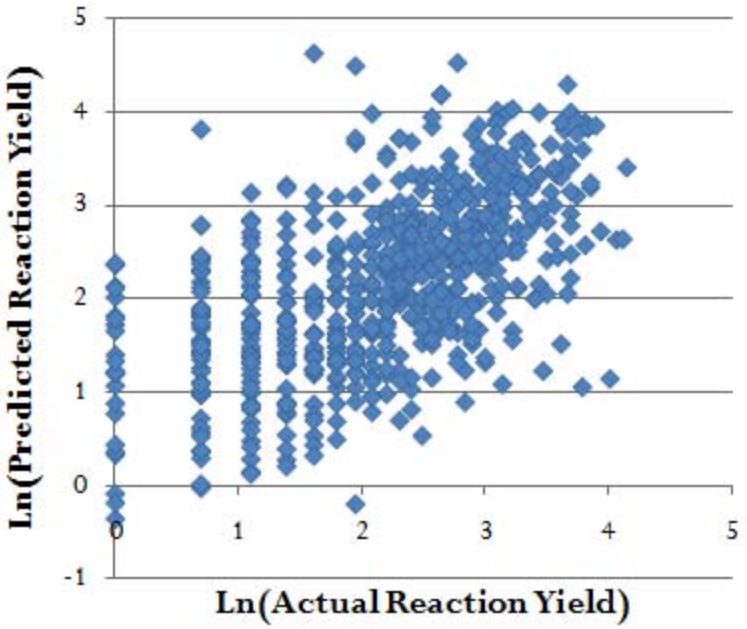
Illustration Problem – Optimizing Reaction Yield



- 7 Different reaction conditions (independent variables)
- 998,400 Possible reaction setups

Data from MacMillan Group. Princeton University

Results



- Estimation can help direct automated synthesis to reaction setups which will likely yield better results.

Data from MacMillan Group. Princeton University

Possible Future Work

- Further work with increasing the reaction yield.
- Estimate various properties for molecular scale solar antennas and other systems. Use these estimates to guide synthesis toward molecules with desired properties.

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