GCEP

Global Climate & Energy Project

STANFORD UNIVERSITY

Rational Organic Semiconductor Material Design
A Pathway Towards Breakthrough Performance in Solar Cells

Investigators
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Objective
The goal of this project is to advance the fundamental understanding of materials design rules for charge and exciton transport, both of which are crucial for organic solar cell applications. To achieve this goal, powerful theoretical tools and characterization techniques will be combined to develop a rational design methodology for novel materials. A feedback loop combining theory, synthesis and characterization will accelerate the discovery of novel photovoltaic materials (Figure 1). This approach will allow development of a systematic path toward identifying promising molecules that will greatly improve the performance and efficiency of organic solar cells.

Figure 1. This project explores the use of strategies from drug discovery, pattern recognition and machine learning in the context of computational materials science to develop donor materials for organic photovoltaics. The goal is to formulate empirical models using a training set of donor polymers with available experimental data for the important current-voltage and efficiency characteristics of candidate molecules. The descriptors are computed, which allows for rapid assessment of key quantities related to the performance of organic photovoltaics for many candidate molecules. As part of the Harvard Clean Energy Project, this approach can be used to quickly obtain an initial ranking of a molecular library with 2.6 million candidate compounds. This method reveals molecular motifs of particular interest, such as the benzothiadiazole and thienopyrrole moieties present in the most promising set of molecules.

Background
Research suggests that thin film solar cells made of copper indium gallium selenide, cadmium telluride and similar compounds will eventually be three-to-five times cheaper to build than conventional solar cells – in part because thin film cells require less material than solid photovoltaic devices and can be easily interconnected on the same substrate. However, there is growing concern that relatively scarce elements, such as indium and tellurium, will be depleted as demand increases for renewable sources of electricity to reduce greenhouse emissions. Organic photovoltaic cells, which can be inexpensively manufactured in high-throughput roll-to-roll coating machines similar to those used to print newspapers, may enable large-scale solar cell deployment for electricity production.

Despite the economic and processing advantages of organic solar cells, laboratory experiments have only recently come close to achieving the 15% efficiency target needed for commercial viability. Creating high-performance organic photovoltaics will require semiconductors with low energy gaps, high exciton diffusion lengths and high charge carrier mobility. A key challenge is...
how to blend all of the requirements in materials with optimized device performance.

**Approach**

This project will address this challenge from a new angle by combining molecular design and device fabrication, theoretical simulation and structural characterization with the large distributed computing power of IBM's World Community Grid (WCG). The WCG distributed computer network permits an 8-hour single-processor calculation to be submitted every 6 seconds – the equivalent of having a 4000-node cluster dedicated to this project (Figure 2).

Instead of testing and manufacturing potential molecular materials, researchers will use the WCG to set up massive numbers of computational calculations to scan through a huge collection of molecular candidates. The results of these theoretical calculations will help determine whether a particular molecule is a suitable match for use in organic solar cells. Specifically, the distributed network will facilitate the prediction of packing structures by molecular dynamics methods, as well as the computation of transfer integrals and reorganization energies for a large number of molecular structures.

![Figure 2](image.png)

**Figure 2.** Screenshot from the Clean Energy Project on the World Community Grid distributed computing website developed by the Aspuru-Guzik laboratory in collaboration with IBM (http://cleanenergy.harvard.edu). The large computational resource provided by the volunteer screensavers of the WCG users will be employed to carry out molecular dynamics calculations aimed at finding the global minimum in the lattice energy of all possible packing arrangements of a given molecular candidate.

Promising candidates derived from the extensive computational search will be synthesized and characterized by measurements of their thin film packing and charge transport. The results derived from the theoretical calculations will be compared against the experimental measurements of both molecular packing and thin film transistor mobilities. These experimental results will be used to fine-tune the theoretical methodologies. Initial theory and experiment feedback loop allowed designing of a new high performance organic semiconductor, showing promise of the above approach.

Following the experimental characterization, promising molecular structures will be integrated into organic solar cell devices to assess their efficiencies. Finally, a database of predicted bandgaps and charge transport parameters for all of the molecules investigated will be created. This information will be publicly available for data mining to select appropriate candidates for organic solar cells or other applications.

**References**


