2010 GCEP Report

Organic Solar Cells

Investigators

PIs:
Zhenan Bao (Chemical Engineering, Stanford University)
Alán Aspuru-Guzik (Chemistry and Chemical Biology, Harvard University)
Michael Toney (Stanford Synchrotron Radiation Laboratory, Stanford Linear Accelerator Center)

Student Participants:
Arjan Pieter Zoombelt (Postdoc)
Anatoliy N Sokolov (Postdoc)
Do Hwan Kim (Postdoc)
Alex Ayzner (Postdoc)
Sule Atahan-Evrenk (Postdoc)
Johannes Hachmann (Postdoc)
Roberto Olivares-Amaya (Graduate Student)

Abstract

In this project, we aim at combining the molecular design and device fabrication expertise of Bao, theoretical simulation expertise of Aspuru-Guzik, structural characterization expertise of Toney, and the large distributed computing power of IBM's World Community Grid (WCG) to rationally design organic semiconductors for solar cells from a completely new angle. Instead of molecular design from intuition, we will combine powerful theoretical tools and various characterization techniques to develop an inverse rational design methodology for novel materials. By doing so, we see a feasible path towards breakthroughs in performance. Such a massive amount of computing resources has not been previously applied to atomic-scale modeling problems in material sciences. For organic semiconductors to find ubiquitous electronics applications, the development of new materials with high mobility and air stability is critical.

Achievement 1: Designed and predicted high charge carrier mobility compounds, realized high charge carrier mobility experimentally: Despite the versatility of carbon, exploratory chemical synthesis in the vast chemical space can be hindered by synthetic and characterization difficulties. We show that *in silico* screening of organic semiconductor materials can lead to the discovery of a new high-performance semiconductor. This work involves the theoretical screening of eight novel derivatives of the dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene semiconductor which has a maximum mobility of 8.3 $cm^2V^{-1}s^{-1}$. Based on the charge transport parameters and the predicted crystal structures, we identified a novel compound expected to demonstrate a two-fold improvement in mobility over the parent molecule. Synthetic and electrical characterisation of the compound is reported with single crystal field-effect transistors, showing a remarkable mobility of 13.7 $cm^2V^{-1}s^{-1}$. This is one of the very few organic semiconductors with mobility greater than 10 $cm^2V^{-1}s^{-1}$ reported to date. More importantly, this is a significant step towards rationally design organic semiconductors for efficient solar cells. For next year program, we plan to extend the theoretical prediction to exciton diffusion length prediction.

Achievement 2: developed a solution processing technique that generated strained organic semiconductor lattice for the first time

For organic semiconductors (OSCs), the molecular packing determines the charge transport of the resulting devices. It is desirable to control the molecular packing of small molecular OSCs through facile processing methods in order to tune the electrical properties of OSC devices. We describe the alteration of the 5,12-bis(triisopropylsilylethynyl) pentacene (TIPSE-pentacene) molecular packing by changing the conditions used during solution processing deposition. Our method deposits TIPSE-pentacene thin film in a non-equilibrium state, and the π-π stacking distance between the molecules can be tuned between 3.08 Å to 3.33 Å as a function of these conditions, which in turn significantly affects the electronic properties of TIPSE-pentacene. The charge carrier mobility was increased from 0.3 cm2/Vs to a record high mobility for TIPSE-pentacene at 4.6 cm^2/Vs. Control of the molecular packing using processing conditions will allow for the development of high performance OSC devices beyond traditional synthetic methods. This is the first time that a π-π stacking distance less than 3.2 Å is realized. Since the charge transport is exponentially dependent on the distance between molecules, such a strained structure is expected to significantly increase the charge transport. This is likely to significantly impact the exciton transport as well, which is the subject of year 2 investigation.

Achievement 3: developed and deployed the computational high-throughput screening on the WCG

In the spirit of the proof-of-principle studies discussed above we have devised the machinery for the large-scale characterization of OSC candidates. We have developed a molecule generator which has produced a primary library of 10,000,000 molecular motifs of potential interest. The quantum chemistry program package Q-Chem was ported to the WCG and we have so far characterized over 1,600,000 million of these oligomer sequences in more than 22,000,000 first-principles calculations. These calculations utilized 3,000 years of donated CPU time. We have set up the server and storage (including a 90TB hard drive pod which we custom built) for the vast influx of results from the WCG. The setup includes a software infrastructure for process automation. Our data collection is used to build up a massive reference database on organic electronics with an emphasis on photovoltaic applications. We have introduced a preliminary empirical calibration of the computed results to bridge the gap between theory and experiment. A first analysis of the current results points to about 25,000 systems with very favorably aligned energetic levels, ideally suited for high-performance OPVs with power conversion efficiencies of 10% or more. Parallel to the first-principles calculations we have been exploring the use of cheminformatics descriptors and ideas from machine learning, pattern recognition, and drug discovery to rapidly gauge the quality of candidates. We have successfully devised initial empirical models for the relevant performance parameters. In the following year we will extend our data mining and analysis capabilities and we will screen for other relevant features and properties in the materials candidates.

Introduction

If the cost of solar cells was reduced by a factor of five to ten, many countries would likely use these to obtain 20% of their electricity from solar energy. If storing electricity also becomes cheaper and rechargeable electric cars are developed, even more electricity would probably come from solar cells and more than a *quarter of greenhouse emissions would be eliminated*. We can reasonably expect that the cost of manufacturing silicon solar cells will drop by a factor of two to three as the industry grows and economies of scale are realized. However, further cost reductions are unlikely because 100-μm-thick wafers of high quality silicon are needed to obtain high efficiency and the wafers must be electrically connected to each other in a batch process.

Many people believe that the thin film cells based on direct band gap semiconductors such as $Cu(In_xGa_{1-x})Se_2$ or CdTe will be three to five times cheaper than today's solar cells because less semiconductor will be used and the cells can easily be connected to each other on the same substrate in an integrated process. There are serious concerns, however, that there is insufficient indium or tellurium to

make as many cells as are needed to generate the 25 TW of power during peak sunlight that is needed to provide an average of 4 TW throughout the day (approximately the amount of electricity needed to make a significant contribution to reducing greenhouse emissions). It is, therefore, very attractive to do research on organic photovoltaic cells (OPVs), which might someday be inexpensively manufactured in high throughput roll-to-roll coating machines similar to those used to make newspapers.

There are many advantages to this approach. Films of organic semiconductors only 300 nm thick can absorb almost all the incident light over a broad wavelength range. There is no shortage of the raw materials needed to make organic semiconductors and they can be deposited very rapidly at room temperature and atmospheric pressure onto plastic substrates. Modules consisting of cells connected in series can be printed in an integrated way. Multijunction solar cells can be made relatively easily since there is no need for crystal lattice matching between layers or high temperature annealing that could cause diffusion between layers. In about 10-15 years, it may be possible to manufacture modules with 15% efficiency at a cost of around $30/m^2$. This capability would truly revolutionize the way we obtain electricity.

We believe tuning molecular packing is the key for controlling the intrinsic exciton diffusion and charge transport properties for organic semiconductors. Additionally, controlling morphology to eliminate structural defects is important for these thin film devices. We will combine the molecular design and device fabrication expertise of Bao, theoretical simulation expertise of Aspuru-Guzik, structural characterization expertise of Toney, and the large distributed computing power of IBM's World Community Grid (WCG) to attack this problem from a completely new angle. Instead of molecular design from intuition, we will combine powerful theoretical tools and various characterization techniques to develop an inverse rational design methodology for novel materials. By doing so, we see a feasible path towards breakthroughs in performance. Such a massive amount of computing resources has not been previously applied to atomic-scale modeling problems in material sciences. However, since its conception, the world distributing computing has been extensively applied in simulating the folding of protein molecules, a problem whose solution required the use of thousands or tens of thousands of today's processors due to the immense number of accessible protein configurations. In this project, we aim to use the distributed computing engine to perform a global optimization of the charge and exciton transport parameters: a costly calculation that would be intractable using traditional computing resources. This methodology will certainly enable us to quickly identify promising molecular candidates to synthesize and test.

Our plans for approaching this problem are distinguished by a continuous feedback loop between experiment and computational modeling. The effort will begin by setting up a massive number of computational chemistry calculations on combinatorial molecular libraries with core structures proposed by Bao (examples shown in later sections). The calculations will be carried out by Aspuru-Guzik employing the WCG infrastructure developed by IBM and harnessed through *The Clean Energy Project*, which was launched by Aspuru-Guzik in December of 2008. The computational power of the WCG distributed computer network allows an 8-hour single-processor calculation to be completed every 6 seconds, which is equivalent to having a 4000-node cluster dedicated exclusively to this project. This facilitates the prediction of packing structures by molecular dynamics methods and the computation of electronic coupling and reorganization energies for a large number of molecular structures by various state-of-the-art electronic structure methods. Promising candidates derived from the extensive computational search will be synthesized and characterized by measurements of their thin film packing and charge transport. Following the experimental characterization, the outstanding molecular structures will be integrated into organic solar cell devices to assess their efficiencies.

Results

See internal report

Progress

The work in year 1 generated new organic semiconductors with close to record-high charge transport properties. This puts us a significant step closer to having materials for high performance solar cells. We still need to rationally design organic semiconductors that have large exciton diffusion length at the same time. This subject is a main focus for year 2 work.

Future Plans

We plan to extend our theoretical approach to exciton diffusion length calculation. We are working on measurements to determine exciton diffusion length with the new materials we prepared in year 1. At the mean time, we are working with new molecular structures designed to meet requirements for solar cells. We are also in the process of fabricating solar cells using the new materials.

Publications

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3) J. Hachmann, R. Olivares-Amaya, S. Atahan-Evrenk, C. Amador-Bedolla, A. Gold-Parker, S. Sanchéz-Carrera, L. Vogt, A. Aspuru-Guzik. The Harvard Clean Energy Project: Large-scale computational screening and design of organic photovoltaics on the World Community Grid. In preparation for submission to *Journal of Physical Chemistry Letters* (2011).

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5) R. Olivares-Amaya, C. Amador-Bedolla, J. Hachmann, S. Atahan-Evrenk, A. Aspuru-Guzik. Descriptor models for organic photovoltaics: What role can simple cheminformatics play in evaluating the quality of complex material candidates? In preparation for submission to *Energy and Environment* (2011).

6) R. Olivares-Amaya, J. Hachmann, S. Atahan-Evrenk, S. Sanchéz-Carrera, A. Aspuru-Guzik. Combinatorial generation of molecular libraries for organic photovoltaics: Exploring chemical spaces via SMILES and SMARTS. In preparation for submission to *Journal of Computational Chemistry* (2011).

Contacts

Zhenan Bao, zbao@stanford.edu

Alan Aspuru-Guzik, aspuru@chemistry.harvard.edu

Michael Toney, mftoney@SLAC.Stanford.EDU

Arjan Pieter Zoombelt, zoombelt@stanford.edu

Anatoliy N Sokolov, asokolov@stanford.edu

Do Hwan Kim, dohwan@stanford.edu

Alex Ayzner, aayzner@slac.stanford.edu

Sule Atahan-Evrenk, sule.atahan@gmail.com

Johannes Hachmann, jh@chemistry.harvard.edu

Roberto Olivares-Amaya, olivares@fas.harvard.edu