

Millions of molecules screened in search for the ideal organic solar cell material

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By screening millions of molecules, researchers hope that the Clean Energy Project will identify a material that can be used to fabricate organic solar cells that have an efficiency of 10-15% and a lifetime of more than 10 years - properties that would make organic solar cells cost-competitive with other energy sources. Image credit: Hachmann, et al. ©2011 American Chemical Society

(PhysOrg.com) -- Currently, the cost of electricity from commercial silicon solar cells is about 10 times higher than the cost of utility-scale electricity. In order to make solar cells cost-competitive with currently available energy sources, some researchers are looking to organic materials. Not only are organic materials less expensive than inorganic

materials like silicon, but they're also non-hazardous, lightweight, easily processed, and can be made semi-transparent and molded into almost any shape. The problem is there are literally millions of organic materials to choose from, and identifying those few that have the best optical and electronic properties is extremely challenging.

To address this problem, a team of researchers from Harvard University, the National Autonomous University of Mexico, and Haverford College in Haverford, Pennsylvania, has developed an extremely large-scale automated computational screening method to study potential molecular structures for organic photovoltaic devices (OPVs). They introduced the initiative, called the Harvard Clean Energy Project (CEP), <http://cleanenergy.harvard.edu/> in a recent issue of the *Journal of Physical Chemistry Letters* where they present some early results, with more studies to follow.

CEP's overall goal is to identify an [organic material](#) that can increase the efficiency of OPVs from the current record of 9.2% to 10-15%, as well as expand the currently limited lifetimes to more than 10 years. A solar cell with these two features could push the power generation costs of organic solar cells below that of other currently available [energy sources](#).

To achieve this goal, the project has taken a highly collaborative approach. It relies on input and feedback from experimentalists from Zhenan Bao's group at Stanford and other research groups. To analyze the large number of molecules, the project combines conventional modeling strategies with strategies from modern drug discovery, along with ideas from machine learning, pattern recognition, and cheminformatics. Also, the project utilizes volunteer computing by IBM's World Community Grid (WCG) to supply part of the large-scale computational power. Volunteers who would like to donate computer time can download a free and virus-free program from the IBM website that uses their computers for screening the materials while their

computer is idle.

“Roughly, every 12 hours of donated free CPU time will result in a new molecule added to our database of candidate organic materials for solar cells,” Alán Aspuru-Guzik of Harvard, who is one of the project’s leaders, told *PhysOrg.com*. “The database will aid scientists in accelerating the discovery of novel solar materials.”

With traditional approaches to analyzing and characterizing materials, researchers typically rely on their past experiences with certain materials and their own empirical intuition. Due to the long time required for synthesis and characterization, only a few examples can be experimentally studied per year. In contrast, CEP can characterize thousands of molecules per day, and the CEP library already contains about 10 million molecular motifs of potential interest.

“The great variety in properties found in our candidate library is quite remarkable, as is the small parameter space that makes for promising OPVs and that has to be hit,” said Johannes Hachmann of Harvard, another of the project’s leaders. “The latter underlines the value of our high-throughput approach.”

Using a calculation hierarchy, the method rates each candidate motif at each step with respect to the desired properties, and expedites further characterization for the most promising candidates. The hierarchy technique is already proving valuable: a preliminary analysis has revealed that only about 0.3% (3,000–5,000) of the screened structures have the necessary energetic levels to realize organic [solar cells](#) with 10% or higher efficiency. While an unaided search would have a very small chance of identifying these molecules, CEP can move all of the promising candidates forward for additional analysis.

“So far, we have made a proof-of-principle study in collaboration with

Zhenan Bao's group at Stanford," said Aspuru-Guzik. "We screened eight different variants of a parent compound for organic semiconductors, and this resulted in a compound with an astonishing large hole mobility. This gives us confidence that the type of approach followed in the WCG will yield useful information to the community."

In addition to searching for molecules with specific structures, the project also gives researchers a better understanding of structure-property relationships of molecules in general. Knowing these design principles will allow scientists to not only improve screening, but also to actively engineer novel organic electronics at a future stage.

"On the one hand, the collection provides on-demand access to specific compounds with a wide range of desired properties and electronic structures for all sorts of applications, not only for OPVs," Hachmann said. "On the other hand it forms a solid foundation to learn about structure-property relationships. Lastly, it will be a useful resource for theoreticians to assess the performance of different computational methods and can serve as a parameter repository in this chemical space."

As more technical results arrive, the researchers are building a reference database that will be available to the public by 2012. The data should accelerate the search for optimal OPV materials, and provide valuable data for the development of organic electronics in general. The researchers hope that one day the search will lead to a clean source of electricity that can compete with conventional energy sources, although it's difficult to predict exactly when that will be.

"In principle, we want the search to last as little as possible," Aspuru-Guzik said. "Obviously, things are more complicated: It takes human time to catalog and understand the results, as well as to select molecules for further screening. We are in the process of selecting the top candidates of our initial screening and releasing them in a publication.

We want to further screen the most promising candidates with more calculations to ascertain and verify their potential as organic solar cell materials.”

To participate and download the client software developed by IBM and Harvard, go to <http://cleanenergy.harvard.edu> and click “Download.” The website contains video tutorials for the installation.

More information: Johannes Hachmann, et al. “The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid.” *The Journal of Physical Chemistry Letters*, 2011, [DOI:10.1021/jz200866s](https://doi.org/10.1021/jz200866s)

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