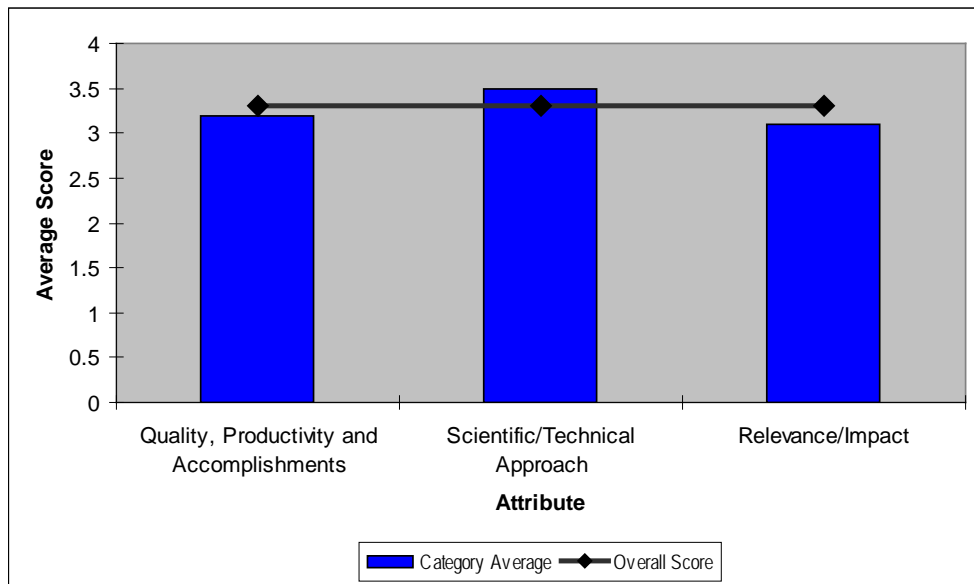


Polymeric Semiconductor Organic PV

Principal Investigator: Brian Gregg, National Renewable Energy Laboratory



Project work in organic semiconductors at NREL. Unique features of the project include its focus on inexpensive, solution processable semiconductors (not vacuum evaporated) and chemically stable materials with a low defect density. Research also includes synthesis of new materials and the employment of purposeful doping (not defect doping) to increase conductivity and minimize interfacial recombination.

Quality, Productivity and Accomplishments (Average Rating 3.2)

Rating Comments

- 3.0 A good start. Team members are leaders in perylene diimide, and related, materials. Synthesis work strong and there is a clear understanding of state of the art benchmarks in OPV. Characterization facilities good. Within the next year, they need also to include stability measurements on cells build thus far.
- 3.0 Objectives: 1) Design and synthesize inexpensive and chemically stable new organic semiconducting polymers without a π -conjugated backbone, 2) Dope one polymer n-type and one p-type with immobile dopants, and 3) Produce efficient doped bilayer OPV cells. These are appropriate exploratory research objectives, which within the context of the materials selection and configuration under development, has the potential to provide disruptive, next generation technology. To his credit, the researcher does not default to the generic descriptions.

Accomplishments: 1) Gram quantities of both new donor and acceptor polymers were synthesized and chemically characterized, 2) n-type and p-type dopants for the two polymers have been synthesized, and 3) Construction of devices and measurement of PV characteristics have been initiated. These accomplishments are aligned with the outlined programmatic objectives, reasonable within the period of performance, and point to a logical progression of materials development.

Qualifications of Research Team and Available Resources: The researcher and his team are well-qualified for the proposed tasks with a demonstrated record of achievement in the areas of technology. He has leveraged a solid history of Office of Science funding to establish a fundamental basis for initial materials selection. The resources available to the research team are appropriate to task.

- 4.0 Excellent team with a long history of generating very precise and thorough measurements from organic materials. Milestones thus far have only encompassed synthesis of a new materials set to enable the experiments and these have been accomplished.
- 3.0 Nice start to an attempt to solve a vexing problem. Interesting new materials have been created, device performance will be the real test and will follow. Gregg and his team are THE people to be doing this.
- 3.0 Substantial initial results, especially the synthesis of novel perylene diimide-based polymers together with their dopants.

Scientific/Technical Approach (Average Rating 3.5)

Rating Comments

- 3.0 Goal of 10% cell good, but perhaps out of reach. Time will tell. The research has been a bit slow, but that's understandable given the new approach of a doped p-n type device (it's more like a homojunction than other OPVs). Their approach is out of the box and bold. That's good. It deserves to be done to see if one can break free of efficiency and stability limitations of most other OPVs. They have a firm understanding of relationship between molecular design and device performance. Stability measurements can be done next.
- 3.8 Dr. Gregg's presentation and report demonstrated good accomplishment towards his project objectives; and a sound fundamental basis for the issues faced for the materials selection task. While desiring both solution processable and chemically stable polymer systems, he has wisely chosen to avoid polymer systems with extensive backbone conjugation. The design motif features saturated flexible linkages between electronically active moieties, and organizing functionalities which would exhibit local ordering. The resulting combination is a novel and organized pathway for electronic communication in the polymer system. Through judicious choice of the active component, the polymer can be doped to be either p- or n-type.
- 4.0 This is an excellent example of the type of hypothesis driven, novel research that is often depressingly absent from the field of organic semiconductors. I have several reservation about whether the idea will work, but the project plan is laid out in such a way that success or failure will be easy to quantify and regardless of whether the (modest) efficiency targets are met we will learn something new about how to manipulate charge separation and electric fields in organic devices. The use of non pi-conjugated materials is a novel departure with reasonable arguments as to why doing so will decrease charge trapping and increase device lifetimes. These sorts of ideas leave the reviewer anxious to see results, regardless of whether he believes the methods will ultimately work.

The exciton diffusion length results for R400 in slide 14 show a great deal of noise. I did not have time to ask about this in the Q&A but it could be indicative of problems controlling the morphology of the R400 polymer. A practical concern is that the efficient separation and transport of charge will require complex control of the dopant concentration profile to maintain enough field across the organic layers away from the interface and the ability to achieve ohmic contacts which may well require another round of doping there. There is some skepticism about whether this degree of control can be accomplished in a solution-deposited system.
- 3.5 The approach of trying to adjust the field in the heterojunction region is a good one. Not clear that this approach will work, but it is definitely "out of the box" in its approach. We all hope that this will work, but have concerns that doping won't solve the problem of recombination, and will require also doping or undoping of the contact regions. Very careful approach – exploratory!
- 3.0 Nice to see alternatives to PCBM. Recombination problem is very important and doping is good

approach to alleviating it. But have we essentially prototyped this work in small molecule devices? See for example, the extensive perylene diimide work by Peumans, et al: Adv. Mater. 2008, 20, 1065–1070. If that work is relevant it does not bode well for the ultimate efficiency of these devices. I'd like to understand better how the PI intends to specifically dope the heterostructure interfaces.

Relevance/Impact (Average Rating 3.1)

Rating Comments

- 3.0 P-N junction may allow OPV to leap over its current limitations. 10% is a reasonable goal in the time frame given. The PI -and all OPV researchers in the DOE program- need to be given a rough cost model (perhaps via simple equations or a set of look up tables or a 'blue book') that can guide material and process selection. This is the most innovative of all the OPV projects in the DOE SETP portfolio. A question, however, arises as to what DOE BES is doing in the field of OPV and if this meshes with the SETP. Here below, I copy the details from the BES web site - *Solar Energy Utilization Research is sought in two major areas: solar-to-electric and solar-to-fuel conversions. Many of the proposed research directions identified in the BES workshop report Basic Research Needs for Solar Energy Utilization (http://www.sc.doe.gov/bes/reports/files/SEU_rpt.pdf) concern important cross-cutting issues, including: (1) coaxing cheap materials to perform as well as expensive materials in terms of their electrical, optical, chemical, and physical properties; (2) developing new paradigms for solar cell design that surpass traditional efficiency limits; (3) finding catalysts that enable inexpensive, efficient conversion of solar energy into chemical fuels; (4) identifying novel methods for self-assembly of molecular components into functionally integrated systems; and (5) developing materials for solar energy conversion infrastructure. BES contacts: Mark Spitler, 301-903-4568, mark.spitler@science.doe.gov; James Horwitz, 301-903-4894; james.horwitz@science.doe.gov; URL: <http://www.sc.doe.gov/bes/SISGR.html>, http://www.sc.doe.gov/bes/reports/files/SEU_rpt.pdf
- 3.2 This work represents a new approach to OPV starting from very stable, inexpensive materials that can be solution cast. The acceptor material (n-type) is based on perylene dianhydride and the donor material (p-type) is a derivative of perylene diimide. These species are synthesized into polymers to enhance their solubility and to improve their film-forming and surface-wetting behaviors. The immediate milestone for the upcoming year is to produce a 4% efficient p-n junction OPV device from these new materials. This goal is rather modest, and this reviewer is not sure whether the emphasis on short term efficiencies for these materials is appropriate. The potential to achieve even higher efficiencies with longer term stability would be more consistent with the exploratory mission of the SETP program. In order to determine the viability of this candidate technology, it is desirable that a strong fundamental basis for the performance of these cells be established, and clear identification of the technical limitations be made.
- 3.0 The phase I efficiency goal of 4% is modest and (if results are to be believed) has already been achieved in other organic systems. The ultimate efficiency targets need to be beyond current state of the art in order, while still grounded in reality, for the practical results of the work to be of high impact. I believe the project will have worthwhile scientific impact regardless of whether it actually achieves high efficiency by the end of its funded period.
- 3.5 Extremely relevant, potentially high impact research, IF it works. We won't know until the data begins to appear, over a wide range of doping and process conditions.
- 3.0 Good fundamental science with potential relevance to the broader organic PV community.

Overall (Average Rating 3.3)

Rating Comments

- 3.0 Preliminary L values are nowhere near where they'd need to be to have a 10% efficient cell unless they have a nanostructured or interpenetrating architecture (known in the literature). The researchers herein need to model this further and address this potential limitation. This project, however, is a research line that could answer (within 2 years) the question of whether OPV and molecular-based PV has any hope.
- 3.2 The presented research plan was clear and exploratory, and if successful could greatly increase the efficiencies of PV devices. Doped polymer systems exhibiting semiconducting behavior are notoriously unstable due to faulty assumptions on the physical properties of conjugated polymers. Dr. Gregg's approach exploits the characteristics of small molecule electronics and liquid crystal organization to propose a polymer pair with greater stability than previously seen. This technology and the accompanying fundamental understanding would make the long term SAI goals more approachable and affordable. The PI has put together a high quality, productive effort.
- 4.0 Very basic science. As many of the Exploratory projects do, it confuses the boundary between BES and EERE funding, suggesting that there needs to be more coordination at the highest levels of DOE between these Offices. A quality project regardless of these issues, which are beyond the control of the PI.
- 3.5 Could be very high impact, must wait and see what kind of device data comes out of this.
- 3.0 I'd be interested to see the PI broaden the goals of the study beyond a pure exploration of one material system. By comparison to PCBM devices, they could also address the secret of PCBM's success, and whether that can be replicated in a lower cost, stable, material system such as the perylenes.