NEBRASKA CENTER FOR ENERGY SCIENCES RESEARCH

Cycle 10
January 2016

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Interface-Engineered Materials For High-Efficiency All-Organics Solar Cells

Abstract.

The proposed project aims to perform exploratory basic research on interface-modified organic semiconductors, to build the foundation for all-organic photovoltaics (OPV) exhibiting efficiencies and stability that are considerably increased as compared to unmodified crystals of organic semiconductors. Starting from archetypical organic semiconductors, P3HT, polyaniline and perylene, and including the recently discovered high-performance organic perovskite organo-lead trihalide, we will seek to improve electron-hole separation through the addition of a molecular dipole layer from *p*-benzoquinone monoimine zwitterions between the semiconductor and the top electrode, to introduce a static electric field that will improve zero bias voltage device performance. Further, the hypothesis is tested that the absorption of light in organic semiconductors generally and the stability of the organo-lead trihalides specifically can be much improved by the addition of and co-crystallization with zwitterions and select dye molecules. The ideal combination of dipolar molecule and organic or metal organic semiconductors for organic photovoltaics will be established from a huge parameter space by a chemical combinatorics approach, which allows for rapid prototyping of materials combinations and is thus compatible with a “Materials-Genome-type” materials design strategy. This project is expected to accelerate a current trend in increasing the photovoltaic efficiency in organics through nanomaterials design, exploiting interface engineering. Project outputs will be a design strategy for interface modified photovoltaic organic thin films, which will be derived from comprehensive data sets on structure and properties of the films, and a all-organics photovoltaic device prototype. These results will enable the PIs to compete for major collaborative grants from NSF, DoE, NASA and AFOSR. The ***impact*** can potentially be huge: the increased photovoltaic efficiency in all-organic materials will enable bendable, flexible, printable materials that could be applied to any surface, including “wearables”, and open unprecedented possibilities for the ubiquitous installation of “green” energy harvesting devices.

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