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Research helps understand factors that influence efficiency of organic-based devices

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Research conducted by Jean-Luc Brйdas, a professor in the Georgia Institute of Technology's School of Chemistry and Biochemistry, aims to understand factors that influence the efficiency of organic-based devices. Georgia Tech Photo: Gary Meek

Organic-based devices, such as organic light-emitting diodes, require a transparent conductive layer with a high work function, meaning it promotes injection of electron holes into an organic layer to produce more light.

Research presented on July 8 at the International Conference on Science and Technology of Synthetic Metals in Brazil provides insight into factors that influence the injection efficiency. A balanced injection of positive and negative charge carriers into the organic layer is important to achieve high quantum efficiency, but the interface between the metallic coating and organic layer where the injection occurs is poorly understood.

Placing an organic layer on top of the conductive layer modifies each layer's individual work function, or the minimum energy needed to extract the first electron from the metal.

"Measuring the work functions independently for each layer does not provide an indication of how their energy levels match when they touch each other," explained Jean-Luc Brédas, a computational materials chemist, professor in the Georgia Institute of Technology's School of Chemistry and Biochemistry and Georgia Research Alliance Eminent Scholar.

The energy levels for each layer should align when attached; otherwise, a barrier will form and a higher voltage will be required to send current in.

With funding from the Office of Naval Research, Brédas first developed a theoretical model of the interface between conventional metals and a single layer of organic molecules forming a self-assembled monolayer on the metal. His goal was to determine how the metal work function could be modified by depositing the self-assembled monolayer.

Brédas and postdoctoral research fellow Georg Heimel, who is now at the Humboldt University in Berlin, looked for changes in the work function of gold when they modified the chemical nature of the head group of the organic molecules in the self-assembled monolayer and the nature of the docking group, which directly connected the organic layer and metal.

The study, published in the April 2007 issue of *Nano Letters*, showed that changing the head group of the organic molecules located far from the surface and changing the docking group provided two nearly independent ways to modify the metal work function.

While studying two metal substrates – gold and silver – the researchers found that even though the chemical interface between the metal and thiol-based self-assembled monolayer were different, the organic-covered metals had virtually identical work functions.

Postdoctoral research fellow Pavel Paramonov, who is now an assistant research professor at the University of Akron, expanded the original work to model the interface between a self-assembled monolayer and indium tin oxide, the conducting material commonly used as the transparent electrode in liquid crystal displays and organic light-emitting diodes.

"Researchers frequently cover the hydrophilic indium tin oxide surface with a self-assembled monolayer containing a hydrophobic subgroup pointing away from the surface, providing much better adherence and compatibility with the active organic layer that comes on top," said Brédas.

The cover layer also prevents the indium from diffusing into the active organic layer and degrading the device, but adding this layer also provides a way to fine-tune the work function.

With funding from the Solvay Group, Paramonov modeled the indium tin oxide surface, which was a complex task because indium tin oxide is not stoichiometric – every vendor's indium tin oxide is somewhat different. Then he modeled the binding of a self-assembled monolayer of phosphonic acid to the indium tin oxide surface. Paramonov's first goal was to determine how the oxygen and phosphorus atoms of the self-assembled monolayer bind to the indium tin oxide surface.

In collaboration with Seth Marder, a professor in the Georgia Tech School of Chemistry and Biochemistry, and Neal Armstrong, a professor in the Department of Chemistry at the University of Arizona, they were able to characterize the main binding modes of the phosphonic acid molecules on indium tin oxide. This work has led to further research characterizing the impact of the self-assembled monolayer on the indium tin oxide work function, according to Brédas.

"More theoretical work needs to be done to study conducting oxides used as transparent electrodes in organic solar cells and organic transistors," added Brédas. "On the experimental side, the quality of the self-assembled monolayer coverage also needs to be improved."

Researchers usually design devices with potentially well-aligned energy levels when the layers are measured individually, but they should be examining the layers when they are attached, according to Brédas. This is because the reorganization of the chemical, electronic and geometric structures of the two layers at the interface has a major impact on the overall device characteristics.

Source: Georgia Institute of Technology

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