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## Improvement of Organic Semiconductor Interfaces via the Diels–Alder Reaction

*Ability to eliminate interfacial problems of organic semiconductors including poor adhesion, thermal expansion mismatch, contact resistance, and metallization damage, through the use of well-defined and mild Diels-Alder reaction*

### Contact

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### Inventors

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### Field

Organic Materials  
Semiconductor Materials  
Materials science  
Passivation  
Adhesion

### Technology

Diels-Alder vapor phase reaction generates new functional groups at the surface of organic semiconductor thin films or crystals. The change of the surface imparts improved interfacial properties to the material.

### Key Features

- Improved adhesion of top contacts, protective layers, or sealants to the organic semiconductor surface.
- Reduced degradation of organic materials through surface layer changes.
- Improved (ohmic) contact at the interface with source and drain.

### Key Benefits

Patent allows a wide variety of functional groups to be appended to an organic surface with greater control over density, location, and other aspects.

### Stage of Development

Chemistry demonstrated. Nature of layer determined. Mechanism understood. Modest optimization of conditions completed. Thermal stability studied. Improvement in adhesion examined.

### Status

Seeking research and development partners.

### Patent Status

Full

### Benefits

The invention exploits the potential for generating well-defined, regular and reproducible surface chemistry using the Diels-Alder reaction. As a result, a single layer of the semiconductor can be altered which generates desired chemical functional groups at the surface, but leaves the bulk properties of the semiconductor intact. Judicious choice of the surface functionalities allows one to reduce or eliminate significant flaws and limitations associated with organic semiconductors. Low energy (poorly adhesive) semiconductor surfaces can be transformed to surfaces with high affinity for metal contacts or any other deposited material. Alignment of energy levels can be tuned via this mild interfacial layer, rather than depending on secondary deposition of buffer layers such as LiF. Reacted surfaces can even replace protective/passivation layers utilized to eliminate metallization damage. In all instances, the reaction method is mild and can be optimized to meet the throughput need of your fabrication line.

### Invention Description

This method doses vapor phase adsorbates onto *polyaromatics*, including *pentacene* and *rubrene*, to achieve the material properties modification described above. The method is applicable to thin films and single crystals. The inventors have demonstrated that a wide variety of functional groups can be appended using this technology. The spectroscopic signatures for the surface reaction match those of fully characterized solution generated equivalents, and thus the chemistry at the surface can be inferred. The process is well understood, proposed mechanisms of surface reactivity exist, rate data is available, and modest optimization of the process has been completed. Standard surface characterization techniques provide details on the composition of the surface and bulk layers. Thermal stability is comparable to or exceeds that of the pristine organic semiconductor.

### Competitive Advantage

The inventors have demonstrated that this new means to react the surface of polyaromatic organic semiconductors via the Diels-Alder reaction can provide the right thrust in creating enhanced-capability semiconductor materials with tailored properties, and thus improve the performance of these materials in electronic applications. The method has additional advantages. In contrast to existing technologies, this method provides a high degree of control over the reaction, to the extent that the coverage control matches/exceeds that found with such high precision techniques such as ALD. Reactions are extremely mild and thus surface coatings can be generated with no damage to underlying substrate. The selectivity of the reaction towards the organic semiconductor means that other exposed elements do not need masking.

### Advantage of Partnership

Industrial adoption is a priority for the inventors and Loyola University Chicago. The inventors are available to assist in the process, via consulting or a research agreement. Most of the impediments and red tape associated with agreements at large research institutions are pleasantly missing at Loyola University Chicago.

### Opportunity

Loyola University Chicago is looking for commercial research and development partners for this technology.



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Associate Professor

B. S., Chemical Engineering, University of Illinois at Urbana-Champaign  
PhD., Chemistry, Rice University

Dr. Jacob Ciszek's research is focused on the interplay between complex synthetic molecules and surface behaviors. He is particularly interested in modulating surface properties, specifically the work function of metals, applying cutting edge synthetic molecules to recently established surface phenomena, and the study of the interfaces between surfaces. His research into the work function of organic materials and semiconductors is targeted at developing more efficient electrical transport mechanisms that could impact applications such as creating more efficient organic light emitting diodes (OLEDs). In addition, he is looking at how classical solution based chemistry can be applied to the surface of non-traditional surfaces such as organic semiconductor crystals and films. His group at Loyola University seeks to take advantage of synthetic chemistry's ability to modify these materials, to improve their performance in devices.