

# Development of Surface Chemistry on-Top of Organic Semiconductor Thin Films to Improve Optoelectronic Devices

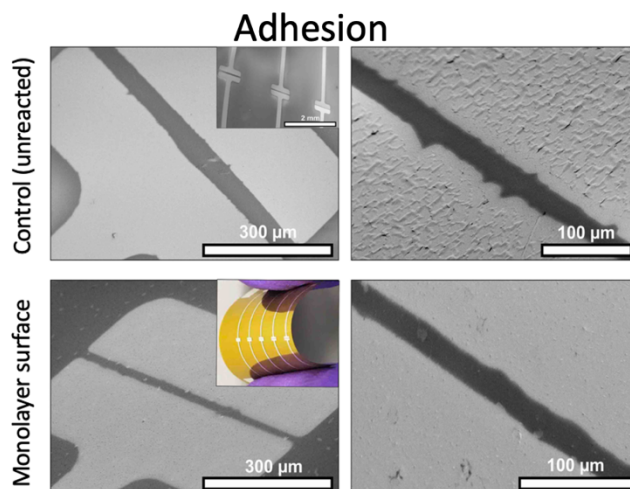
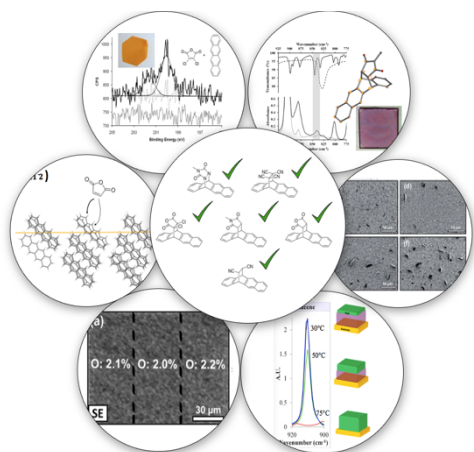
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Organic devices (OLED, OFETs, OSCs) are commonly configured such that a metal contact must be deposited on top of the organic semiconductor. These interfaces often suffer from numerous flaws including poor adhesion, metal penetration, poor surface wetting (discontinuous films), and significant charge injection barriers. We feel that the ability to selectively change the surface of the organic layer via chemistry would allow for improved interactions with the deposited metal and, in-turn, improve device performance. Vast literature shows monolayers (deposited on top of gold, silicon, etc.) can address many of these issues when the system is reversed (organic on metal), but the methodology for installing them is inapplicable to organic thin-films. This points to an obvious need for controllable surface chemistry on top of the organic semiconductor.

We have developed click-like” Diels-Alder chemistry that allows prototypical OFET films (tetracene, pentacene, rubrene) to be appended with a variety of small molecules to form an interfacial layer only ~1 nm thick. The reacted surface is highly tailorable with dozens of combinations explored for a variety of application. This basic approach is presented in detail. This work then summarizes many of the expected and unexpected deviations which occur due to the very unusual nature of the organic surface, namely its high anisotropy, recessed reaction loci, and weakly bound molecular units. Concluding the fundamental components, we highlight some of our recent work in generating analogous chemistry on OLED electron transport layers, specifically TPBi.

This work concludes by highlighting many interfacial components the chemistry aims to improve, focusing primarily on the morphological and mechanical structure of applied metal top contact. Specifically, we examine how the various functional groups improve surface wetting of the metal, film continuity, adhesion in flexible contacts, metal penetration, and sheet resistance.

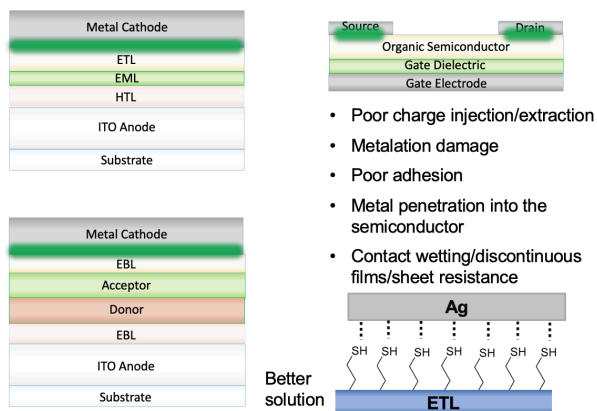


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## Supplementary Pages

First, I just want to make sure the problems we aim to solve are clear. An additional image showing the prominence of the metal on organic interface (green in figure) is usually helpful in that regards.

### Across all Three Systems, Problems Originate at Interfaces



Overall, I try to highlight some of the more interesting aspects of the chemistry. This is, after all, a very different approach to improving this interface. At the same time I understand that this audience is more interested in the application. With the latter in mind, there is an emphasis on the range of molecules and thin-films, monolayer characteristics, the application processes and limitations. An example figure on the novelty is shown below. Here a crystal of tetracene has completely different reactivity (as shown by the Cl 2p XPS signal) on the two faces, which can be justified based on the molecular packing at the surface of the crystal

Highlighting some of the materials from the application side, reaction cause dramatically changes to the metal wetting and lesser changes to the degree of penetration. Film continuity unsurprisingly improves and sheet resistance drops appreciably.

Most of the images have been removed due to the restrictive file size.....

The presentation would pick the highlights the following references from my group and work that is in preparation for publication.

*Chem. Mater.* **2021**, *33*, 9515

*CrystEngComm.* **2020**, *22*, 4108

*Chem. Comm.* **2019**, *55*, 13975.

*RSC Advances.* **2019**, *9*, 26942.

*J. Phys. Chem. C.* **2018**, *122*, 15582.

*Langmuir* **2017**, *33*, 8140.

*CrystEngComm.* **2016**, *18*, 6062.