

## PCSI

### Room Ballroom South - Session PCSI-TuM2

#### Organic and Hybrid Semiconductor Materials & Interfaces

Moderator: Wanyi Nie, Los Alamos National Laboratory

##### 11:00am PCSI-TuM2-31 Development of Surface Chemistry on-Top of Organic Semiconductor Thin Films to Improve Optoelectronic Devices, *Jacob W. Cizek*, Loyola University Chicago

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.

##### 11:05am PCSI-TuM2-32 Characterizing Nanopattern Formation of Polymer Thin Films on Silicon Substrates with Ion Beam Sputtering, *Jocelyn Zhang*, Boston University, Del Norte High School; *G. Pettis*, Oregon State University, Boston University; *B. Jiang*, Boston University, Turkey; *N. Baker*, Boston University; *E. Guney*, Sabanci University, Turkey; *G. Ince*, Sabanci University IICEC, Turkey; *K. Ludwig, Jr.*, Boston University

Surface nano-patterns formed by ion beam sputtering (IBS) have been reported by many research groups with most focus on semiconductor and metal materials [1]. However, limited study has been conducted on polymer nanopatterning introduced by IBS [2]. This study aims to understand polymer film wrinkling in relation to ion beams and humidity conditions, which could potentially introduce effective methods of tuning chemical and physical characteristics of polymer film surfaces. Poly(4-Vinylpyridine) (4-VP) and Polystyrene (PS) polymer thin films on silicon substrates were sputtered with Ar<sup>+</sup> ions under ultra-high vacuum (UHV) and then placed in either humid or dry conditions. The results show that wrinkling patterns are formed in 4-VP film after sputtering at 2 keV and consecutive humidification, but no wrinkling patterns are observed in PS under the same condition. The wrinkling amplitude of 4-VP films increases over time under humidity. Areas of lower ion flux have less order and higher amplitude wrinkling in 4-VP. Increasing film thickness increases wrinkle wavelength and decreases the order in the wrinkles. It is also found that the surface contact angle with water increased on both 4-VP and PS after ion beam sputtering, presumably due to increased roughness.

##### 11:10am PCSI-TuM2-33 Functionalizing Organic Semiconductors with Dipole Monolayers, *Matthew Williams*, Loyola University Chicago

This work seeks to improve OFETs performance via the addition of a chemisorbed monolayer on top of the organic material to address various issues such as contact resistance and charge trapping. The monolayer is made possible via site-specific Diels-Alder chemistry which only reacts with the semiconductor. By installing specific functional groups to the surface, the aforementioned issues can be eliminated, resulting in improved charge injection and/or charge transport in organic material.

We focused on the addition of monolayers which contain significant electronic charge separation (or molecular dipole) within their structure. This feature can act as a potential step, shift the mean energy in gaps, and/or align energy levels between materials. We first utilize the chemistry to selectively append dipole-containing molecules to trap states at grain boundaries for polycrystalline OFETs in order to shift the mean energy within the grain boundary and improve device performance. Grain boundaries are unavoidable flaws inherent to the materials, and the ability to address trap states would be a powerful way to address these flaws post-fabrication. This performance improvement is exemplified in conductance measurements with two orders of magnitude increases, improved threshold voltages, and doubling of mobility.

Additionally, we can optimize the surface potential of thin films by systematically varying similar dipole-containing monolayers. A linear relationship between dipole strength and surface potential shift is seen, as predicted by the Helmholtz equation. The achieved potential adjustments are attributed to the monolayer and result in a high degree of tunability of surface potential. With the capability to shift potential up to ~800mV, reducing electron charge injection barriers is hypothetically feasible. The challenges arising in conductance measurements are discussed.

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