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# Understanding the chemical and electronic properties of OLED materials


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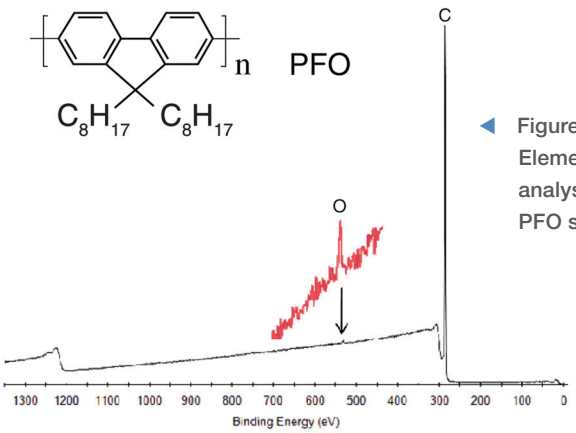
## Key Words

ESCALAB, Band Gap, OLED, REELS, Surface Analysis, UPS, Valence Level, XPS, Nexsa

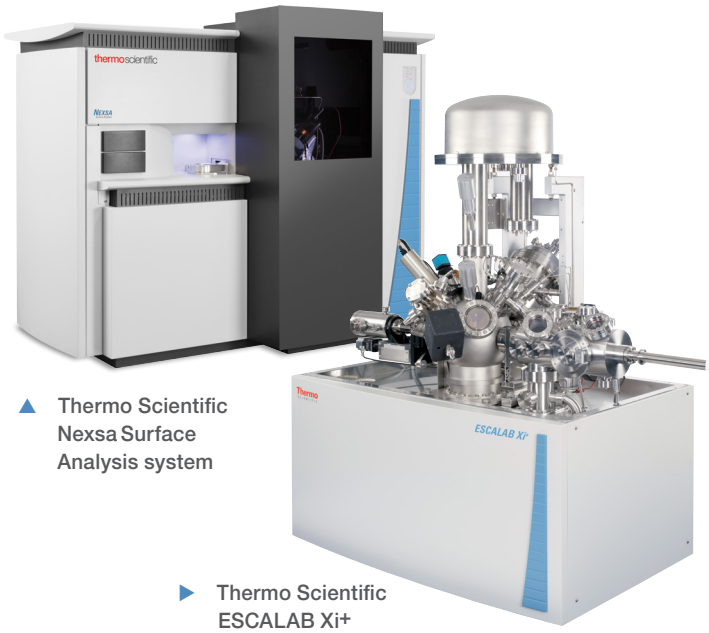

A component material for an OLED was analysed to understand the surface chemistry, and determine the energy level plot based on analysis of the HOMO and LUMO states.

## Introduction

Organic LED (OLED) displays are expected to be the future of the display industry. OLED displays typically draw less power than the displays currently available on the market. As a result, portable screens would be able run for longer from a single battery charge. One OLED material is poly (9,9-dioctylfluorene) or PFO. PFO is a high brightness, blue-light emitting material with a low turn-on voltage. It has a large optical gap,[1] however, and that means that in order to make the most of its potential for OLED displays, the overall design of the OLED device has to be carefully developed and controlled to prevent any adverse interaction with charge carriers in PFO films.




◀ Figure 1: Elemental analysis of PFO surface




▲ Thermo Scientific Nexsa Surface Analysis system

▶ Thermo Scientific ESCALAB Xi+

To understand the interaction of PFO with charge carriers, it is necessary to understand the electronic structure of PFO itself. This requires a multitechnique analytical approach. Thermo Fisher Scientific offers XPS instruments, such as ESCALAB and Nexsa, which can be configured with multitechnique options, allowing much of the electronic structure of PFO to be investigated with a single tool.

## Experimental and results

A 30 nm PFO film was deposited onto a glass substrate and analyzed after being stored in a fluoroware container for several days. The analysis was done on Thermo Scientific™ ESCALAB™ Xi+, which can be configured with various options for multitechnique analysis and sample preparation. XPS elemental analysis of the PFO surface (Figure 1) showed a small amount of oxygen (0.6 at%) at the film surface. PFO itself only contains carbon (hence the strong carbon peak in the spectrum) so the observed oxygen must be a contaminant deposited onto the surface during storage or transit. Detailed chemical analysis of the carbon was

carried out using high energy resolution XPS (Figure 2). In this way, XPS could be used to measure the surface purity of PFO films. The strongest peak in the spectrum is due to core-level transitions in the aromatic and aliphatic carbon of the PFO polymer. Small peaks due to valence transitions in the PFO are also observed. These peaks contain information that is needed if the full electronic structure of PFO is to be understood, but the peaks are relatively weak and they are convoluted with core-level peaks. Using a multi-technique approach, however, we can analyze these valence transitions more easily.

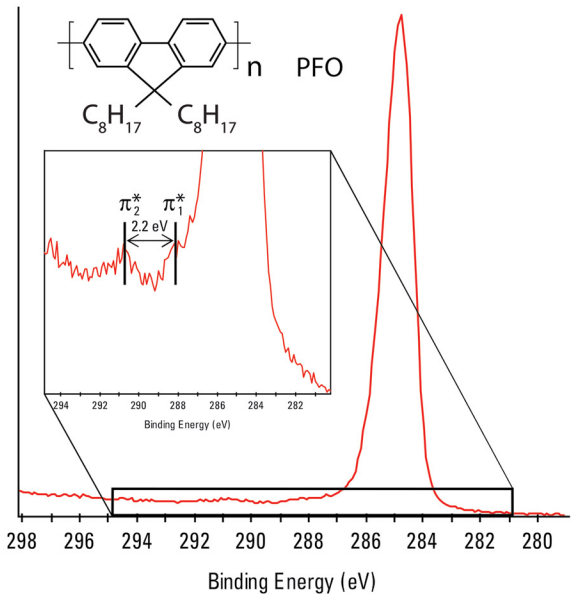



**Figure 2: High resolution C1s XPS spectrum of the surface**

Most Thermo Scientific XPS tools, including ESCALAB, offer reflected electron energy loss spectroscopy (REELS) as standard. This technique, which measures the electrons from an incident beam scattered by the top surface, is the ideal technique for investigating carbon aromaticity and unsaturation. The valence levels of aromatic polymers can be studied without interference from core-level carbon transitions. Additionally, the technique is extremely surface sensitive and it is possible to obtain information from the top 1 nm of the surface.

An example of REELS data from a high quality polystyrene film is shown in Figure 3. Polystyrene has a long aliphatic polymer backbone with phenyl side groups: each phenyl group is chemically identical. The REELS spectrum shows a single sharp peak at 6.6 eV and a broad hump at around 20 eV. The broad hump is due to interaction of the primary electron beam with lattice plasmons, but of more interest in this work, the sharp peak is due to $\pi$ to $\pi^*$ transitions in the aromatic valence levels. A single peak reflects the single chemical environment of the phenyl groups.

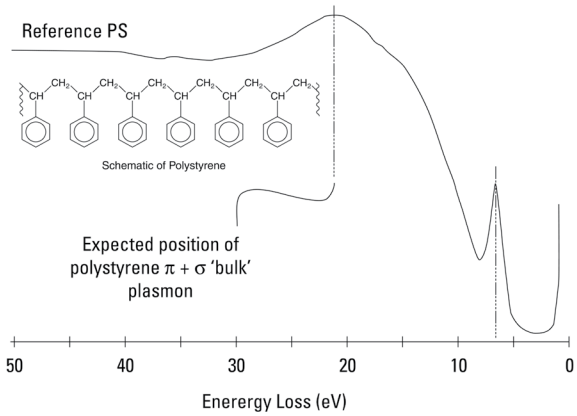



**Figure 3: REELS spectrum of polystyrene film**

REELS analysis of PFO in Figure 4 shows two $\pi$-$\pi^*$ peaks, presumably from the two different aromatic bonding environments of the 5 and 6 membered carbon rings. These peaks are due to the same transitions that cause the small peaks in the carbon XPS spectrum but they are not convoluted or obscured by core-level transitions. The $\pi$-$\pi_1^*$ peak at 3.7 eV energy loss is due to valence transitions from the highest occupied bonding $\pi$ level to the lowest unoccupied $\pi^*$ anti-bonding level. The energy separation between these levels is therefore 3.7 eV. The second peak is due to transitions from the same $\pi$ level but to a higher lying $\pi^*$ level, some 2.2 eV above the lowest unoccupied level. This information concerning the energies of these peaks will be used later on to measure the band gap of the PFO film.

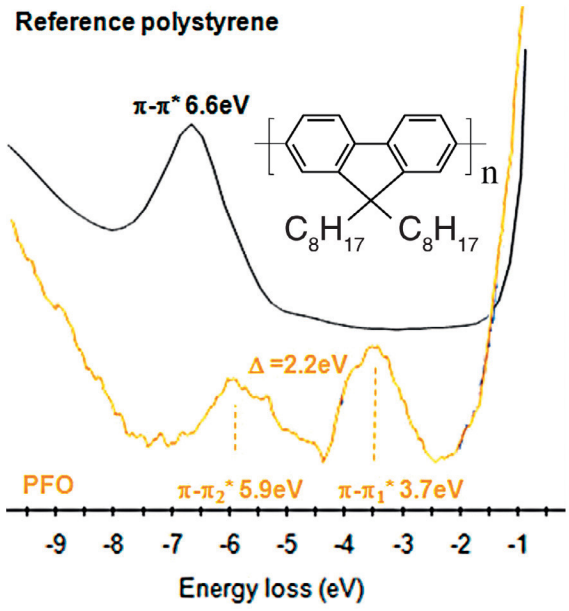



**Figure 4: UPS spectra of polystyrene and PFO**

Further information on the valence levels of the PFO was obtained with ultraviolet photoelectron spectroscopy (UPS). UPS uses a helium discharge source, which has a significantly lower energy than the monochromatic aluminium K-$\alpha$ X-rays used for XPS, making it ideally

suited for investigating valance band transitions. Using UPS it is possible to measure the ionization potential of OLED films, and as well as many other valence level parameters (Figure 5). In particular, since the Fermi level position can be determined from UPS of a gold sample, it is possible to measure the energy of the highest occupied molecular orbital directly from the UPS data. This molecular orbital is identical to the π-bonding level involved in the π-π* transitions observed in REELS.

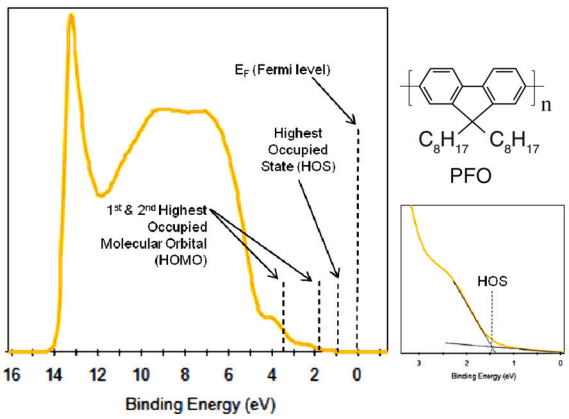



Figure 5: UPS spectrum of the valence level of PFO material

As the energy of the π-level is known from UPS and the REELS data gives the energy gap from this level to the π* levels, the energy level diagram (or electronic structure) of PFO can be created. With this diagram, it is then straightforward to calculate a band gap of 3.3 eV for PFO which agrees with the published value.[1] Information about the valence electronic structure is needed if optimal PFO-based OLED devices are to be made. To make OLED devices, the PFO would be doped with other materials to adjust and control band structure, changing the light emitting characteristics of the device. Using the multi-technique approach shown for undoped PFO, the electronic structure of doped films could be analyzed and characterized.

## Summary

The performance of OLED-based devices depends on the chemical and electronic properties of the materials used. By using a multi-technique approach, we have shown how scientists and engineers can characterise candidate OLED materials, detect contaminants on the surface, and understand how their electronic structure affects their operation.

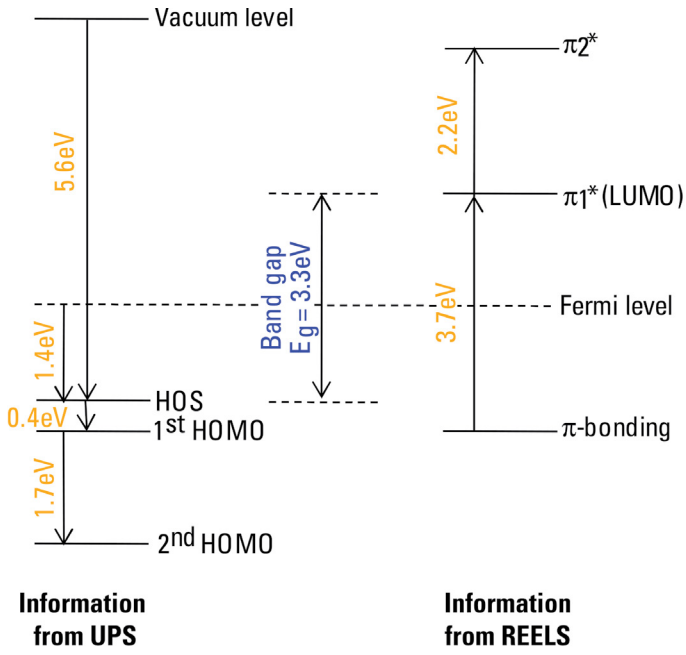



Figure 6: By combining the information from REELS and UPS the energy level diagram of PFO surface can be created

## Acknowledgement

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## References

1. L. S. Liao, *Applied Physics Letters*, Vol. 76, No. 24, 12 June 2000

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