Soft X-ray spectroscopy study of molecular semiconductors for durable organic photovoltaics.

Project title:	Soft X-ray spectroscopy study of molecular semiconductors for durable organic photovoltaics.
PRISMAS Research Area:	Clean Energy
Supervisor:	Ellen Moons
Hosting University:	Karlstad University
Partners:	James O'Shea, Nottingham University
Link to position:	Apply here

1. Project summary:

Organic solar cells (OSC) have recently reached power conversion efficiencies up to 18% mainly thanks to the synthesis of new high-performance electron-donor molecules and non-fullerene electron-acceptor molecules. The remaining challenge is to increase the lifetime of OSCs. Photodegradation, in particular photo-oxidation in presence of oxygen and water vapor, of the molecular semiconductors that make up the photoactive layer is a major concern.
To study the photo-induced degradation of the components, we will, first, study intentionally exposed solution-coated thin films of selected conjugated molecules and their blends to simulated sunlight in air for increasing lengths of time. The changes in composition and electronic structure will be measured by valence band and core-level photoelectron spectroscopy (XPS) and near-edge X-ray Absorption Fine structure (NEXAFS) spectroscopy at C1s-, N1s-, O1s and other relevant X-ray absorption edges, as well as by resonant photoelectron spectroscopy. The latter is a unique technique to probe the contributions of specific parts of the molecule to the valence band structure, which is available at the FlexPES beamline at MAX IV. The 2D resonant emission maps will reveal which moieties are affected by the photodegradation, providing guidelines for the design of more photostable materials.
Secondly, we will use ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) to follow selected degradation processes in-situ in controlled gas (mixture) environments. For this purpose, we aim at using an ambient pressure beamline, such as SPECIES at MAX IV. In-situ measurements will reveal the degradation kinetics and its dependence on the environment.
The outcome of this study will contribute to a better understanding of the electronic structure of these state-of-the art molecular semiconductors and the photodegradation mechanisms that limit the operational lifetime of OSCs. This understanding will provide guidelines for mitigation of photo-induced degradation and pathways towards more durable organic solar cells.

2. Keywords

Solar energy, Photovoltaics, Sustainable energy, Durable electronic devices, Molecular Materials, XPS, NEXAFS, Res-PES.

3. Project outline

- **State of the art:**

Co-funded by the European Union

Organic solar cells (OSC) have recently reached power conversion efficiencies up to 18% mainly thanks to the synthesis of new high-performance electron-donor molecules and non-fullerene electron-acceptor molecules. The remaining challenge is to increase the lifetime of OSCs. Photodegradation, in particular photo-oxidation in presence of oxygen and water vapor, of the molecular semiconductors that make up the photoactive layer is a major concern. Therefore, this project aims to unravel the photodegradation mechanisms of the new high-performance materials for organic solar cells, using soft X-ray spectroscopy techniques.

- **Project objectives:**

To study the photo-induced degradation of the components, we will, first, study intentionally exposed solution-coated thin films of selected conjugated molecules and their blends to simulated sunlight in air for increasing lengths of time. The changes in composition and electronic structure will be measured by valence band and core-level photoelectron spectroscopy (XPS) and near-edge X-ray Absorption Fine structure (NEXAFS) spectroscopy at C1s-, N1s-, O1s and other relevant X-ray absorption edges, as well as by resonant photoelectron spectroscopy (Res-PES). The latter is a unique technique to probe the contributions of specific parts of the molecule to the valence band structure, which is available at the FlexPES beamline at MAX IV. The 2D resonant emission maps will reveal which molecular moieties are affected by the photodegradation, providing guidelines for the design of more photostable materials. For this study a two-month secondment at the MAX IV Laboratory's FlexPES beamline is envisaged during the first year of the project.

Secondly, we will use ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) to follow selected degradation processes in-situ in controlled gas (mixture) environments.

In preparation of this second secondment at MAX IV, an additional two-month secondment in the group of Professor James O'Shea, Nottingham University, UK, will be offered in the second year of the project, providing the opportunity to carry out ambient-pressure (AP) experiments using a lab-based AP-XPS instrument with integrated solar simulator. These lab-based tests of photodegradation of molecular semiconductor films will be carried out in-situ under simulated sunlight, in the presence of different gases. These preliminary experiments will allow us to select the most interesting samples to study in more detail with high-resolution XPS experiments at SPECIES at MAX IV. Preliminary results will also strengthen the beamtime proposal and increase the chance to be granted beamtime at SPECIES.

Finally, we envisage a two-month secondment during the third year of the project during which we plan to use the ambient pressure beamline SPECIES at MAX IV to study selected samples with XPS in different environments. In-situ measurements will reveal the degradation kinetics and its dependence on the environment. It will also allow us to distinguish between processes that occur at different rates at different sites on the molecule.

The outcome of this study will contribute to a better understanding of the electronic structure of these state-of-the art molecular semiconductors and the photodegradation mechanisms that limit the operational lifetime of OSCs. This understanding will provide guidelines for mitigation of photo-induced degradation and pathways towards more durable organic solar cells.

- **References:**

Examples of earlier work of the research group on photodegradation of organic solar cell materials and performance of all-polymer organic solar cells without fullerene derivatives can be found in the following references.

1. *The Photooxidation of $PC_{60}BM$: New Insights from Spectroscopy,* Iulia Brumboiu, et al., Phys. Chem. Chem. Phys. 24 (2022) 25753. DOI: 10.1039/D2CP03514F.
2. *Impact of intentional photo-oxidation of a donor polymer and $PC_{70}BM$ on solar cell performance,* Vanja Blazinic, et al., Phys. Chem. Chem. Phys. 21, 40 (2019) 22259. DOI: 10.1039/c9cp04384e.
3. *Over 14% efficiency all-polymer solar cells enabled by a low bandgap polymer acceptor with low energy loss and efficient charge separation,* Qunping Fan, et al., Energy & Env.Sci.**13**, (2020) 5017. DOI: 10.1039/D0EE01828G.

Link to PRISMAS overview: https://www.maxiv.lu.se/prismas/