EU COST Action MP1307 – Unravelling the Degradation Mechanisms of Emerging Solar Cell Technologies

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***Abstract*—Organic and hybrid perovskite based solar cells have a huge potential to significantly contribute to a clean electricity supply of the future. However, so far they exhibit complex and hierarchical degradation paths and their understanding can only be acquired through the application of complementary chemical and physical characterization techniques. This limited device stability is the main hurdle for a successful and large scale market introduction of these emerging solar cell technologies. Our StableNextSol Action has created a highly interdisciplinary network of laboratories, as well as corresponding industry, overall more than 120 partners, with complementary analytical techniques for the study and understanding of the degradation mechanisms occurring in state-of-the-art devices. Our Action integrates and generates fundamental knowledge and expertise to foster disruptive innovations targeted to mitigate device failure and to propose and develop new concepts for more stable solar cells. Value is added to the entire value chain of photovoltaic research at European and international level, as well as variety decision makers in the public sector by supporting specialisation policy**

and standards still lacking in this research field. The outcome of the Action will contribute to resolve the global challenges facing the industry and this COST Action initiative has brought together all these expertises and resources to promote the cooperation between different sectors, academia, public authorities and industry.

Keywords—COST Action; solar cell; photovoltaic; stability; organic solar cells; perovskite solar cells; degradation mechanisms

I. Introduction

Organic photovoltaic devices (OPVs) and Pervoskite Solar Cells (PSCs) have major potential as a principal source of clean electricity for the future. However, the large-scale introduction of OPVs and PSCs onto the market is currently limited by their stability. The Action StableNextSol[1] has created a highly interdisciplinary network of academic and industry researchers to study the degradation mechanisms occurring in state-of-the-art OPVs and PSCs, based on the use of complementary analytical techniques.

This Action, chaired by Prof. Monica Lira Cantu and running since March 2014, integrates and generates fundamental knowledge and expertise to foster disruptive innovations targeted to mitigate device failure, and aims to develop new concepts for OPVs and PSCs that are more stable and reach lifetimes longer than 20 years.

II. Objectives of the Action

The principal objective of the Action StableNextSol is to take advantage of the different and complementary analytical techniques and knowhow available within the wide network of academic, institutional and industrial partners of the consortium to study and understand the degradation in state-of-the-art OPVs and PSCs. The objectives are split into scientific/technical objectives and networking objectives.

A. Scientific/Technical Objectives

- Fabrication of solar cells and test structures.
- Following ISOS protocols[2] for the degradation/stability analysis of OPVs and PSCs.
- Applying a wide range of characterization techniques to study degradation.
- To elucidate degradation mechanisms in detail.
- To consolidate degradation mechanisms into “families” or “groups”.
- Developing models to simulate the degradation behavior of OPVs and PSCs.
- Proposing disruptive alternatives to reduce or eliminate the degradation paths in OPVs and PSCs.
- Fabrication of next-generation OPVs and PSCs with enhanced lifetime.

B. Networking Objectives

- To establish a multidisciplinary network of research laboratories.
- To create long-term collaborative teams.
- To train the next generation of research scientist experts on OPV and PSC stability.
- To encourage the participation of female researchers.
- To unify protocols on OPV and PSC degradation.
- To apply for Horizon 2020 projects.

III. Participants

The StableNextSol Action has brought together over 430 researchers from 136 institutions, 18 of which are industries.

The participants in StableNextSol come from:

- 29 COST countries (Belgium, Bosnia and Herzegovina, Croatia, Cyprus, Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Ireland, Israel, Italy, Lithuania, Malta, Netherlands, Norway, Poland, Portugal, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey, United Kingdom)
- 2 Near Neighbour COST countries (Belarus, Russia)
- 2 International Partner COST countries (China, USA)

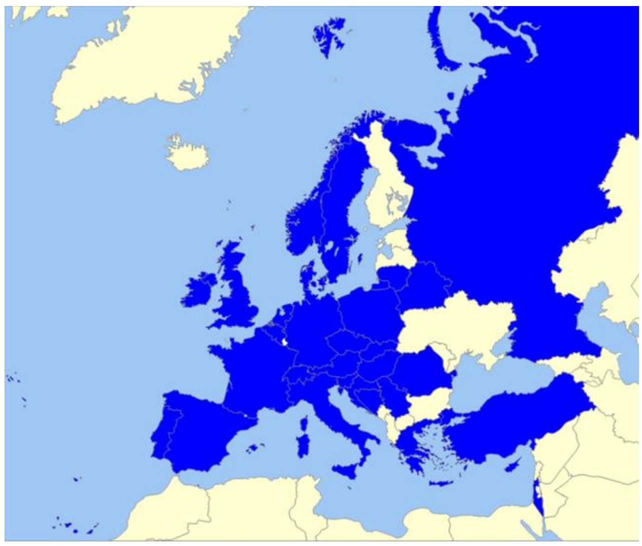

Fig. 1. Participant Countries in the StableNextSol COST Action MP1307: 29 COST Countries, 2 Near Neighbour COST countries and 2 International Partner Countries (China, USA, not shown).

IV. Working Groups

A. WG1 - Technology Monitoring

Specific objectives for this WG led by Dr. Nieves Espinosa are monitoring the latest advances in the field of emerging solar cell technologies to ensure the network is working within the state-of-the-art and finding distinctive degradation patterns that have a positive impact on these fields. To achieve this objective, a collaborative activity consisting in creating an up-to-date database that collects all data published about degradation is ongoing. A literature review is complementing this database containing further details.

Objectives

1. Materials and device configuration

An OPV device consists of several different organic materials that are sandwiched between inorganic electrodes and can be configured in various ways. A PSC has a similar structure, but the photovoltaic active layer is consisting of organic-inorganic hybrid perovskites and often TiOx is used instead of organic transport layers. For the planned experiments materials and the device configuration are defined for all partners based on state-of-the-art devices. As more and more materials for OPV and PSC are synthesised and other device configurations are developed, new materials developments concerning active layer and charge transporting interlayers will be monitored in order to make sure that the consortium is working on state-of-the-art materials and industrially-relevant challenges. Another objective of this WG is to find general degradation patterns distinctive for a certain material or family of materials combining the knowledge of the Action and latest reports in literature. Special focusis given to those new materials with the possibility to meet the requirements of next generation OPV and PSC devices, these are, materials that can give high photovoltaic performance, synthesized through green chemistry and easily processable, and most importantly, intrinsically stable.

2. Degradation protocols and industrial requirements

Degradation protocols and standards are applied in accordance with the current ISOS recommendations[2] and future IEC standard(s). As evolution in the testing conditions is expected during the course of the Action, the technology monitoring will also focus on any breakthroughs in accelerated testing methods, degradation protocols and standards evolving in the field. The insight into the requirement for industrial application of OPVs and PSCs is gained through regular networking events and industrial days as well as from technology and industrial reports.

3. Characterization methods

If any new characterization technique becomes known that is very useful for studying degradation, it will be included within this Action at specific partners' institutions or by inviting new members.

Main deliverables

The main deliverable of WP1 is to be constantly aware of the most recent advances in OPV and PSC materials, characterization methods and device development. An overview of the latest development is included in the annual reports.

B. WG2 - Solar Cell Fabrication

Initially, WG2 focused only on OPV, but the results from WP1 indicated early one that it is mandatory for our action to also include PSC, which have seen a remarkable progress in recent years with significant potential for clean energy conversion. Hence, this WG is currently divided into two sub-groups, one devoted to OPV fabrication (Dr. Yulia Galagan) and a second one devoted to PSC fabrication (Dr. Francesca Brunetti), but general approach of each subgroup is similar.

Objectives

1. Device fabrication

The fabrication of state-of-the-art devices is being carried out by specialized member laboratories that have the facilities to continuously provide a large enough number of comparable samples for all partners, e.g. TU Ilmenau (university) or the Heliatek GmbH (industry). For selecting the device structure advice from the industrial associates and the WG1 has been paramount and the device fabrication is ongoing..

2. Test structures fabrication

In parallel to fully working OPV and PSC devices, comparable test structures consisting of a few layers are made in regular intervals. This test structures are aged and analysed in parallel to understand interfacial mixing, reaction and degradation. The recommendations from experts in characterization in WG4 are the basis for the test structures.

Main deliverables

The main deliverable of this WG is to provide reproducible and large number of devices and test structures to the partners for the different degradation scenarios and, thereafter, non-destructive and destructive analysis.

C. WG3 - Solar Cell Degradation

Ageing OPV and PSC in a reliable and comparable way is a challenge due to the many different influences that affect the degradation behavior of those emerging solar cells. This WG led by Dr. Sjoerd Veenstra ensures that all devices and test structures are degraded to well controlled and documented conditions such that reliable interpretation can be drawn from the collected results.

Objectives

1. In-situ degradation of OPVs and PSCs

In-situ degradation of OPV and PSCs is continuously being carried out on state-of-the-art devices. Several sets of samples are being monitored, from reference devices to degraded devices at different, but well-defined, exposure times and conditions.

2. Degradation protocols

Following well-established degradation protocols for indoor and outdoor testing, sets of systematically prepared

OPVs, PSC and corresponding test structures are made and distributed to the partners for in depth degradation analysis with all complementary methods. The ageing experiment follow at the moment the ISOS recommendations[2]. Degradation protocols are continuously evaluated and will be extended and improved after agreement of all the partners, Management Committee (MC) and Science & Technology Group (SG). The main existing degradation protocols that are being used are:

a) *Real-Time Outdoor Ageing – ISOS-O-3*

b) *Indoor High Temp. Light Soaking – ISOS-L-2*

c) *Indoor Humidity Light Soaking – ISOS-L-3*

d) *Reference Dark Storage Shelf Life – ISOS-D-1*

e) *High Temperature Dark Storage – ISOS-D-2*

f) *Damp Heat Storage – ISOS-D-3*

g) *Temperature Cycling Test – ISOS-TC-3*

h) *Low Light Testing – ISOS-LL*

Main deliverables

The main deliverable of this WG is to ensure that device degradation and testing OPVs, PSCs and test structures follows relevant protocols and standards. The WG delivers systematically aged devices and test structures to WG4 and WG5, which focus on the characterization of those samples.

D. WG4 – Non-destructive Characterization

Non-destructive chemical and physical characterization mechanism offer an important piece in the puzzle to develop a microscopic material degradation – physical parameter – device failure relationship. Non-destructive analyses allow the samples to be characterized by several means and by different expert groups without destroying the devices. This is a big advantage, since the same OPV and PSC can be characterized by different and complementary analytical methods before these devices return to WG3 for continuation of their ageing process. This work is led by Dr. Harald Hoppe.

Objectives

1. Comparison of the qualitative and quantitative device degradation of samples that are aged in parallel at different groups is paramount for StableNextSol. One challenge that is currently being overcome is the lack of data standards in the field of OPV and PSC by developing interchangeable data formats, e.g. building on the FMF format[3].

2. The second objective is to establish relevant and available characterization techniques and their sequence for efficient characterization for analysis of devices aged in WG3. WG1 is also contributing to this objective to leverage latest advances in characterization and avoid investigation of recently discovered failure paths.

3. Non-destructive characterization of devices and test structures at different stages of their degradation are being carried out successively or in parallel at different laboratories. Techniques to be considered for non-destructive testing include standard optoelectronic characterization of the OPV performance, in combination with imaging techniques to reveal the location of any failures. Chemical and surface and bulk structural characterization techniques of test structures allow for a better understanding of the failure on the material level. These are successfully being combined with physical and spectroscopic techniques to link the failure to physical parameters.

4. Some characterisation tools are available at nearly every partner, but some of the specialist tools are not only available at few locations but additionally they are often time-consuming and costly. Therefore the selection of relevant samples by the experts in WG3 and WG4 is crucial.

5. Degradation can occur at different locations within the device, for example the light adsorbing layer, the electrodes, the many interfaces between layers, etc. Due to such complex structure and diverse degradation paths the application of modelling and simulation approaches is very important for the future advancement of the technology. In this respect, modelling and simulation is being used as a tool to understand OPV and PSC lifetime and results is being compared with experimental data obtained from the non-destructive and destructive analyses.

The results of the different characterization methods are step by step combined to aim at global understanding of the different degradation paths taking place in devices and test structures. This implies using the results both from non-destructive methods (in this WG) and destructive methods (WG5) and comparing them to other reports in the literature.

Main deliverables

The main deliverable is being able to describe the degradation mechanisms based on the large number of results obtained within the non-destructive analyses, with the aim at generalizing the finding for other materials and device structures. Suggestion to prevent these degradation routes and possible ways to derive accelerate testing methods for these particular processes. Results obtained in this WG will be combined with those observed in WG5 in order to arrive to more comprehensible degradation mechanisms.

E. WG5 – Destructive Characterization

As described for non-destructive characterization, the destructive chemical and physical characterization is the second main piece in the puzzle towards understanding of the relationship between the microscopic material degradation, the physical parameters and the device failure. In this case, as measurements cannot be repeated, many samples, of the same characteristics, have to be degraded at the same time since the samples are destroyed for final characterization. This WG is led by Prof. Eugene Katz.

Objectives

1. Destructive characterization techniques is using to large extent those samples submitted to non-destructive techniques, but also samples dedicated solely to this WG. These measurements are carried out at different laboratories in parallel. Destructive techniques enable to detect degradation at

buried interface and in the bulk by relying on tools that than sputter in parallel to the analysis. The tools that are currently available allow analysing structural and interdiffusion processes on cross-sections applying microscopy techniques, like transmission and scanning electron microscopy (TEM and SEM, respectively). Change in chemical composition or oxidation state of the compound as well as interdiffusion processes are X-ray photoelectron spectroscopy (XPS) and Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS). Impact of interdiffusion and changes at the interfaces on the mechanical strength of the devices are measured using double cantilever beam (DCB) tests. These tools are only available at few locations and they are often time-consuming and costly. Therefore, as before, the experts in WG3 and WG4 always ensure selection of the most relevant samples.

2. Modelling of the opto-electrical response of the degraded devices is implemented combining exiting device modelling expertise and insight about the degradation mechanisms. The characterization techniques in WG4 generates parameters such charge carrier mobility, excited state lifetime and diffusion length, energy levels, etc. that are direct input for the simulation. The modelling aims to validate and complement the understanding extracted in WG5.

3. Experimental results generated in WG5 also enable the modelling of the chemical interactions, material diffusion and other processes in the device during degradation. This can assist the understanding of the failure at the microscopic level. It furthermore contributes to prediction of device performance behaviour at different stress levels which can be the foundation for accelerated lifetime models.

Main deliverables

To describe the different degradation mechanism observed by destructive characterization analyses is the main deliverable of this WG, as well as to compare the opto-electrical modelling of device degradation in order to experiment results and discussion of relevant differences. Furthermore, we will suggest how to prevent these degradation routes and possible ways to derive accelerate testing methods for these particular processes. As also described for non-destructive analyses, the results obtained in this WG are being combined with those observed in WG4 in order to arrive to more comprehensible degradation mechanisms.

F. WG6 – New Device Engineering

Eventually, this COST action aims at developing new, longer lasting devices, which is the focus of this WG led by Dr. Tom Aernouts.

Objectives

1. Design the next generation stable OPVs

The first ideas on the design of the next generation stable OPVs have been developed, taking into account results from other WGs, especially WG4 and WG5. Regular brainstorming exercises are taking place during the MC meetings, with special focus on industrial partners' input to arrive at innovative and industrially-relevant solutions for the problems encountered.

2. Simulation and Modelling

The new devices are validated through modelling and simulation in order to predict the best device configuration and the novel OPV lifetime.

Main deliverables

The main goal of WP6 and a key deliverable of StableNextSol is to deliver stable OPV and PSC devices based on the knowledge gained within all other working groups such that these technologies can fulfil their technological and societal potential. Fabrication of the next-generation of OPV devices is foreseen, and these are fed back into the production and characterization scheme starting with WG2 in an iterative scheme to further learn from those new devices and improve them further.

V. ACTIVITIES

In parallel to the scientific and technologic program there is a networking program ensuring that the involved partners are working close and closer together, building the a multidisciplinary network and creating long-term collaborative teams. These activities are led by Prof. Elizabeth von Hauff.

A. Meetings

The Action organized two meetings every grant period and will continue to do so. These meetings comprise a MC Meeting and a meeting of the WG. Additionally, at least one of the meetings also includes a Topical Conference and/or an Industrial Day. The following events were held so far, including two upcoming events:

Grant Period 1:

- MC/WG Meeting & ISOS7, Barcelona, Spain, October 2014
- MC/WG Meeting & Symposium E at the E-MRS, Lille, France, May 2015

Grant Period 2:

- MC/WG Meeting, Vilnius, Lithuania, October 2015
- MC/WG Meeting & Conference "New trends in solar cells, Bratislava, Slovakia, April 2016
- MC/WG Meeting & ISOS8, Freiburg, Germany, October 2016

B. Short Term Scientific Missions

A core component of our StableNextSol COST Action is the short term scientific missions (STSM), which are administered by Prof. Koen Vandewal. These STSM are an important component in training the next generation of research scientists in this multidisciplinary field During the course of this project, the following STSMs were awarded.

Grant Period 1: 19 STSMs awarded

Grant Period 2: 23 STSMs awarded

More information can be found on: http://stablenextsol.eu/activities/short-term-scientific-missions/granted-stsms/

C. Training Schools

To exchange experience with other networks and build a stronger research base for Europe, we co-organised a training school with the ITN Establis[4]

- ESOS Training School, Cargèse, France, 4-11 June 2015

D. Dissemination

Since the start of this COST action, more than 11 publications were published in internationally renowned, peer-reviewed journals, with many further publications in the pipeline. Further means of disseminating the results are our Industry Days as well as the website[1] and webinars. These efforts are coordinated by Dr. Marta Fonrodona and Dr. Antonio Urbina.

Due to the dissemination of the project results, the StableNExtSol Action has grown from 47 participants from 18 COST countries at the point of submitting the proposal to currently more 430 participants from 27 COST countries.

Acknowledgment

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References

[1] http://stablenextsol.eu

[2] M. Reese et al., Sol. Energy Mater. Sol. Cells 5, p1253-1267 (2011) http://dx.doi.org/10.1016/j.solmat.2011.01.036

[3] M. Riede et al., Comput. Phys. Commun. 3, p651-662 (2010) http://dx.doi.org/10.1016/j.cpc.2009.11.014

[4] http://www.project-establis.eu/