Abstracts Book

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Influence of Electrode Degradation on Organic Solar Cells Functioning – a Computational Study

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Recently, organic solar cells (OSC) have reached the efficiency of 10% becoming a reliable alternative to the conventional high cost inorganic solar cells. However, to gain a place in the competitive market of solar cells it is necessary to improve their lifetime. Due to the nature of the materials used, there are several degradation mechanisms [1] that lead to a decrease on device efficiency and thus to its failure, being of upmost importance to understand how they affect organic solar cells functioning. One of these mechanisms consists on electrodes degradation when in contact with air or water, leading to a change on electrode work function and thus of the energy levels at electrode/organic layer interface. As a result, the decrease on OSC efficiency has been attributed to a loss on the electrode´s ability in collecting charges from the active layer [2, 3]. However, it is unclear how a change on electrode's work function affects the main optoelectronic mechanisms that rule the device performance [4], which can give some guidelines to prevent its failure. In order to clarify this issue we performed computational experiments with our improved mesoscopic model. Our results show that changing electrodes work function affects simultaneously all optoelectronic mechanisms that rule exciton and charges dynamics, and thus the device performance.

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INFLUENCE OF ELECTRODE DEGRADATION ON ORGANIC SOLAR CELLS FUNCTIONING – A COMPUTATIONAL STUDY

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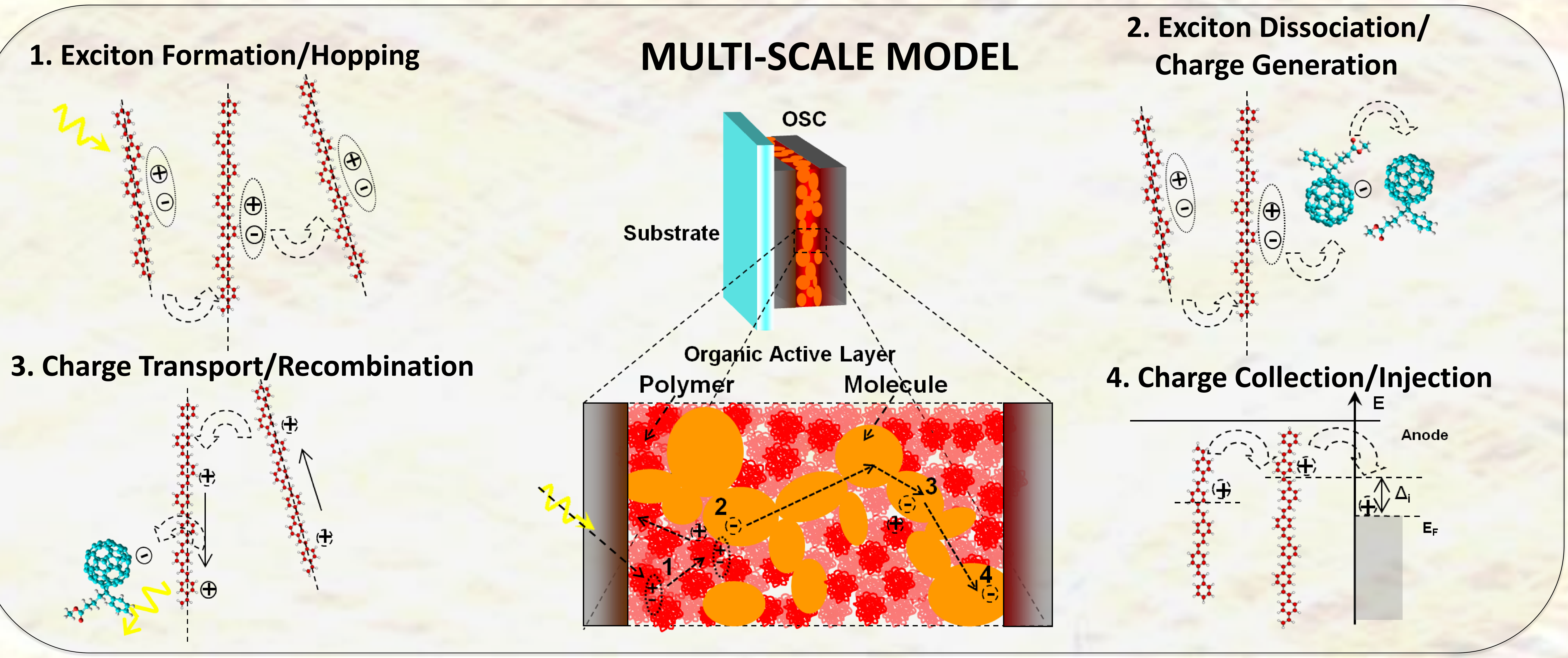
Recently, organic solar cells (OSC) have reached an efficiency of 12% becoming a reliable alternative to the conventional high cost inorganic solar cells. However, to gain a place in the competitive market of solar cells it is necessary to improve their lifetime. Due to the nature of the materials used, there are several degradation mechanisms [1] that lead to a decrease on device efficiency and thus to its failure. One of these mechanisms consists on electrode degradation, leading to a change on its work function. As a result, a decrease on OSC efficiency has been attributed to a loss on the electrode ability to collect charges from the active layer [2, 3], being unclear how changes on electrode's work function affects the main optoelectronic mechanisms that rule the device performance [4]. To address this issue we performed a computational study using the mesoscopic model for OSC developed by us.

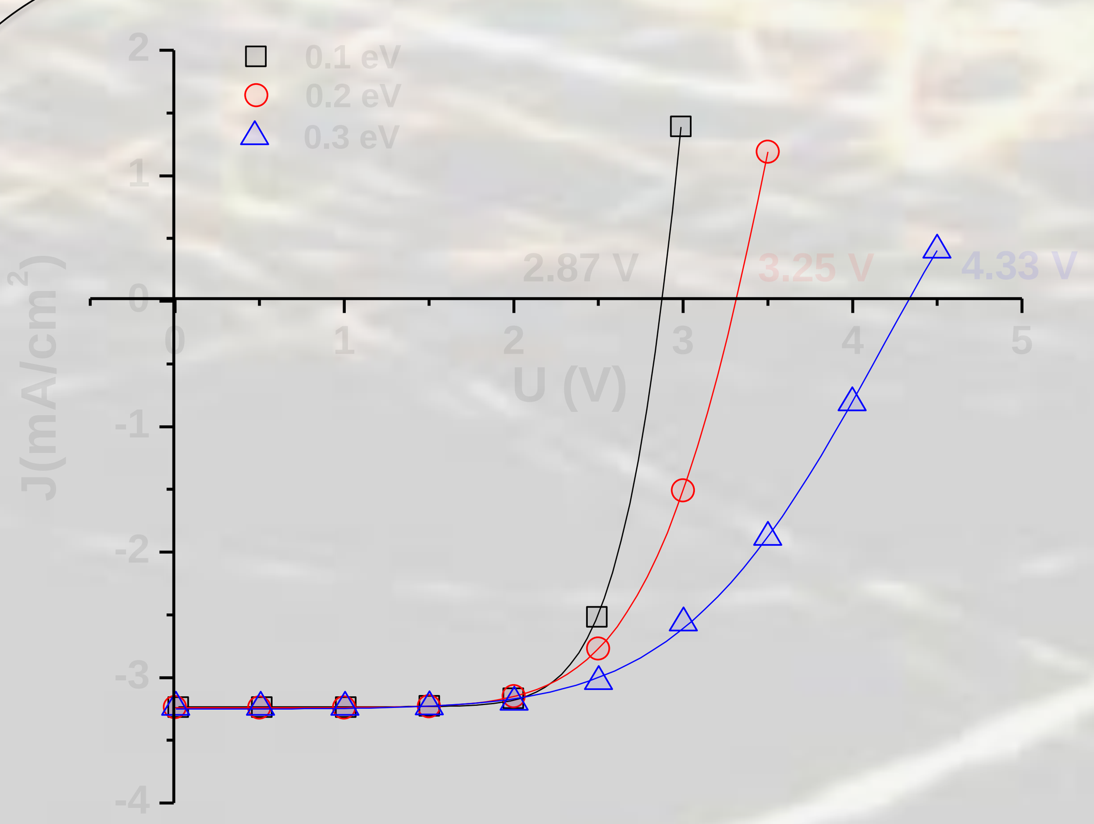
MULTI-SCALE MODEL



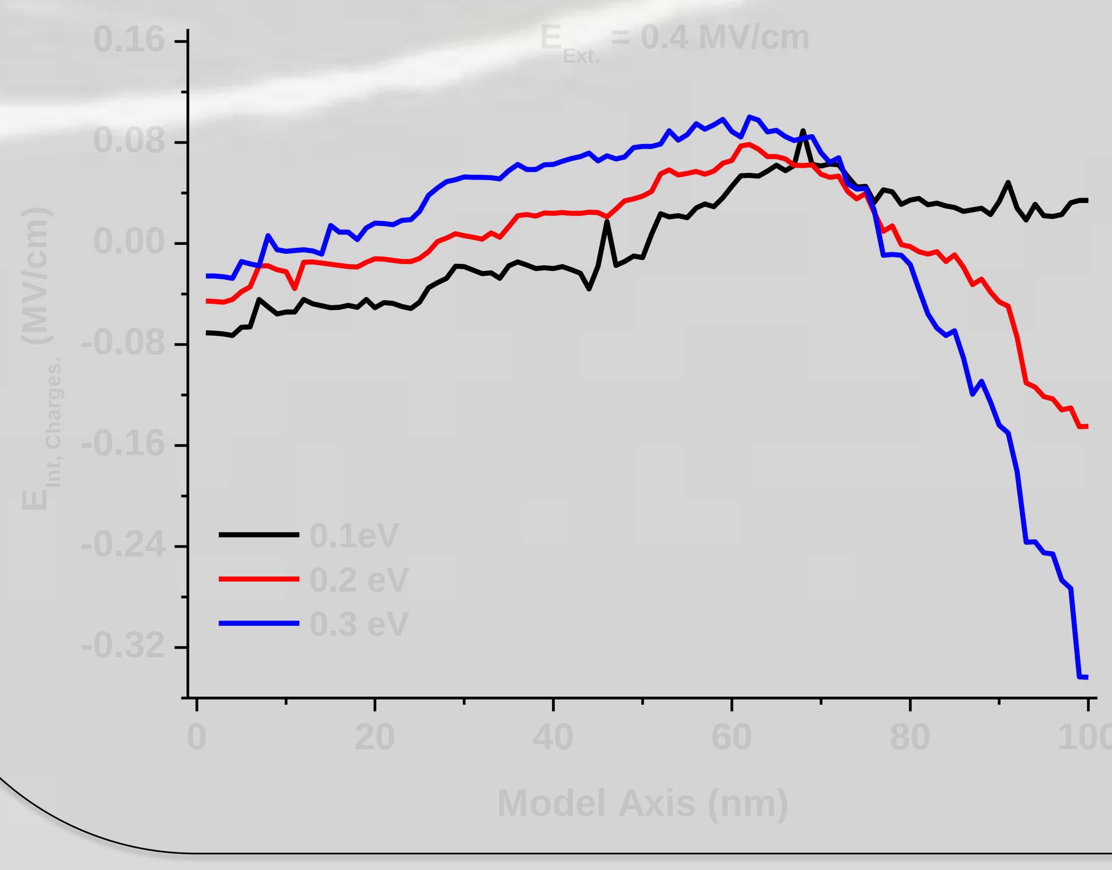
Simulation Conditions:

- *Poly*(*p-phenylene vinylene*) (**PPV**)/Phenyl-C61-butyric acid methyl ester (**PCBM**) (20:80), being the molecular properties obtained by quantum MD calculations.
- Dark current and under ilumination was obtained by changing Δi, and thus eletrode's work function.
- E_{ext} was changed from 0.0 MV/cm to 0.45 MV/cm, allowing to extract I vs V curves and thus J_{sc}, V_{oc} and **FF**.

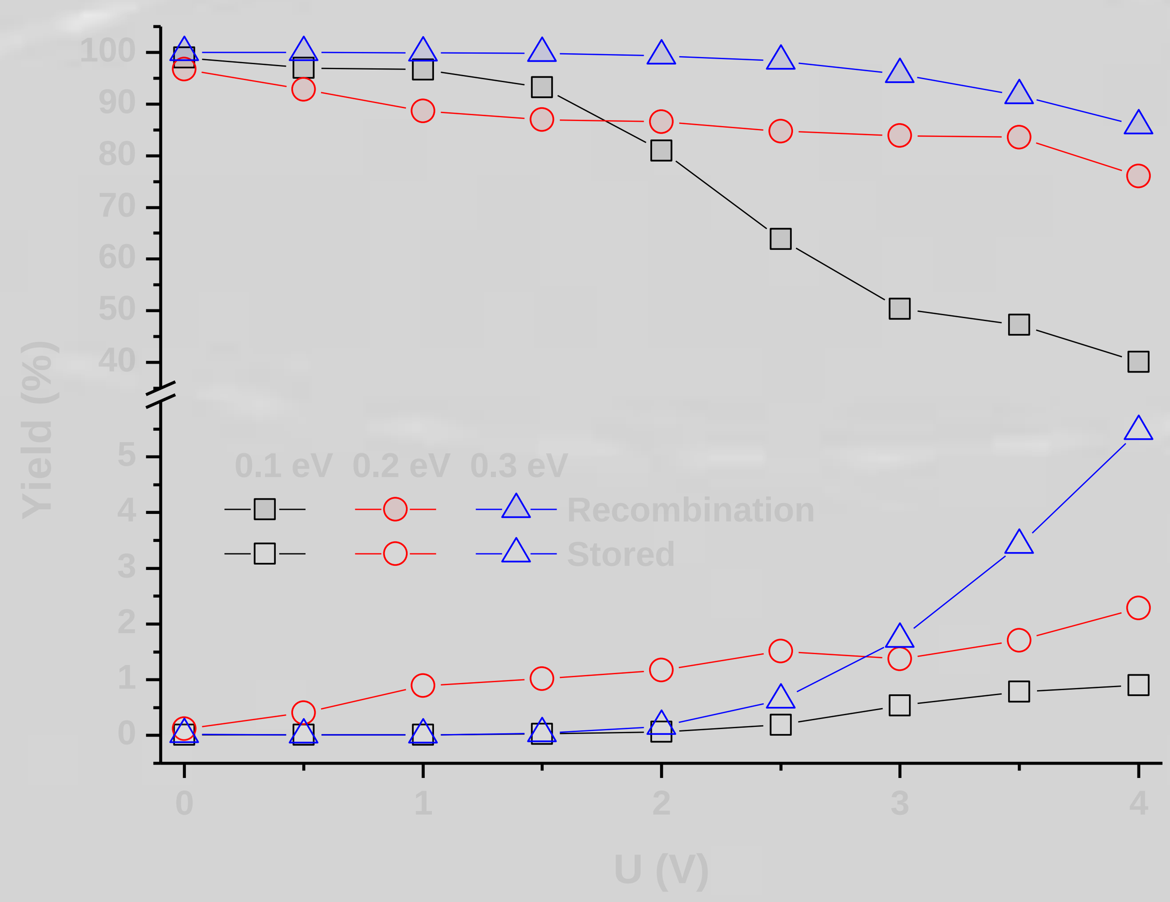
RESULTS AND CONCLUSION



- The increase of the energy barrier (i.e. eletrode degradation) at the active layer/eletrode interface (from 0.1 eV to 0.3 eV) increases the open circuit voltage (from 2.87 V to 4.33 V).
- The changes on the I-V curves due to eletrode degradation leads to a decrease on the field factor (FF = 74.1 % for 0.1 eV to FF = 67.2 % for 0.2 eV to FF = 55.8 % for 0.3 eV).
- No changes on the short circuit current is observed.



- Above hinders charge collection, eletrode degradation leads to an increase on the amount of charge stored and the charge that undergoes recombination.
- As a result of the charge stored distribution inside the active layer, there are significant changes on the internal electric field induced by these charges mainly near the anode.



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