Impact of SAM's on Photogenerated Carrier Dynamics at Perovskite Interfaces

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Keywords: *perovskite, self-assembling monolayers, photocurrent dynamics, photovoltage transients*

Abstract:

Self-assembled monolayers (SAMs) on hole-collecting electrodes in p-i-n perovskite solar cells can effectively replace traditional bulky hole-transporting layers.[1] Yet, the exact mechanisms by which these monolayers influence electronic processes, and how these effects depend on the monolayer molecular properties, remain unclear.
In this work, we designed a simplified perovskite device with blocked electron extraction to study photocurrent dynamics at the perovskite/ITO interface. Using short laser pulse excitation, we analyzed photoluminescence and photovoltage responses to compare bulky and monomolecular hole transport layers. Our findings show that photovoltage dynamics are strongly influenced by the properties of both the transport and perovskite layers, which vary depending on sample preparation methods. The photocurrent dynamics arise from multiple processes, including charge displacement in the local electric field, hole transport to the ITO, hole trapping at interfacial states, and electron-hole recombination.
We present a model considering molecular dipole moments and ionization potentials to explain the varied effects of different monolayers on hole extraction and recombination rates. Furthermore, the photovoltage dynamics exhibit pronounced memory effects persisting for minutes to hours, attributed to ion redistribution under illumination.

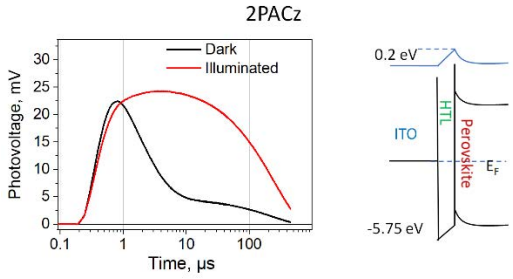

Figure 1*: Photovoltage transients measured at ~10 nJ/cm^2 excitation intensity in different samples nonexposed to constant light (black lines) and immediately after the sample illumination for 30 seconds by ~1 Sun light (red lines). Images on the right-side show energy diagrams evaluated by accounting energy levels of ITO, perovskites and hole transporting materials. The numbers in energy diagrams indicate ionization energies of hole transporting materials (bottom numbers) and increase of vacuum energies (as well as increase of apparent ITO work function) caused by dipole moments of SAMs (top numbers) evaluated from data of ref. (DOI: org/10.3390/molecules29091910) Equilibration of Fermi levels causes up-bending of perovskite energy bands.)*

Conflicts of Interest

Please declare that there is no conflict of interest.

References

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