UNVEILING PHOTOLUMINESCENCE QUENCHING MYSTERIES

Davide Regaldo [a], Thomas W. Gries [b,c], Valerio Stacchini [c], Jean-Paul Kleider [d,e,f], Antonio Abate [b,c], Artem Musiienko [b]

[a] *Center for Nano Science and Technology @ PoliMi, Istituto Italiano di Tecnologia, Via Rubattino, 81, Milan, 20134 Italy*
[b] *Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Berlin, Germany*
[c] *Department of Chemistry, University of Bielefeld, Bielefeld, Germany.*
[d] *IPVF, Institut Photovoltaïque d'Ile-de-France, 18, Boulevard Thomas Gobert, 91120 Palaiseau France;*
[e] *Université Paris-Saclay, CentraleSupélec, CNRS, GeePs, 91192, Gif-sur-Yvette, France;*
[f] *Sorbonne Université, CNRS, GeePs, 75252, Paris, France.*

Among the multitude of characterization techniques, transient (Tr) and steady-state (ss) photoluminescence (PL) asserted themselves as powerful tools for probing optoelectronic properties, carrier recombination dynamics, and the performance of semiconductor devices, owing to their contactless, purely optical nature.

Despite the ubiquity of PL, there is still no consensus on the correlation between PL features, such as amplitude and decay time, and device performance: are the former good predictors of the latter? In other words, if a modified structure shows a decrease in PL intensity with respect to the reference (PL quenching), does this imply that this structure is yield to lower-quality or better-quality solar cells? Even more tricky is the analysis when PL is performed on half-cell structures, where the absorber layer is deposited onto a selective carrier transport layer (SCTL) due to the intricate problematics of carrier recombination vs carrier extraction. As a matter of fact, this half-cell structure is very often used for characterization purposes.

To explore this issue, we choose metal halide perovskites (MHPs), a maturing photovoltaic technology which has been extensively characterized with Tr and ss PL, and we focus on MHP half-cells. We complement the analysis with the help of another technique that is sensitive to the spatial separation of carriers, namely transient surface photovoltage (TrSPV).

Previously, we deposited MHP thin films on doped and co-doped TiO_2 layers, and a drift-diffusion (DD) model has been tuned to reproduce TrSPV measurements on the two charge extraction layers [1]. Here we employ the calibrated model to study the impact of charge extraction and carrier recombination on PL intensity, TrPL decay, and TrSPV. Our findings show that PL quenching is obtained for both enhanced carrier extraction, as well as increased non-radiative recombination at the MHP/SCTL interface. Beyond this, we reveal the root cause of PL quenching upon charge extraction, and we show the sensitivity to other parameters in our DD simulations.

Starting from our findings, we establish a comprehensive protocol for reliably analyzing PL spectra. Furthermore, providing a deeper understanding of the charge carrier extraction mechanisms in MHPs, our work paves the way for a fast optimization of semiconductor devices, thereby advancing the fields of physics, optoelectronics, material science, and chemistry.

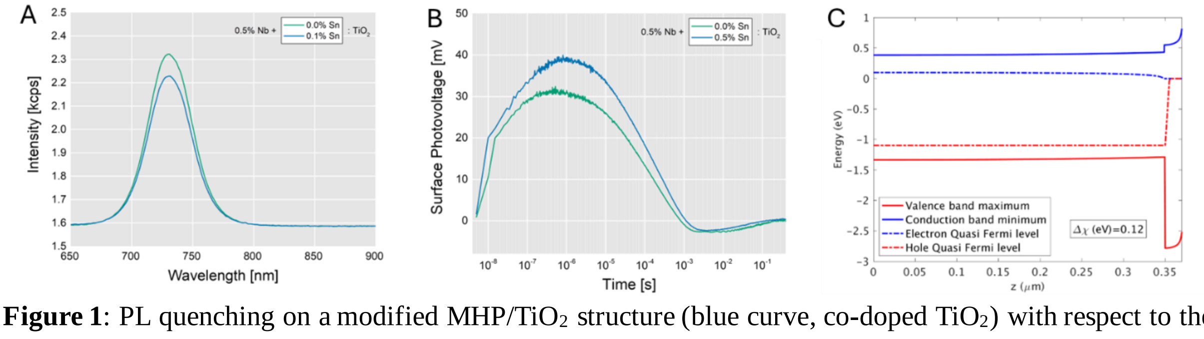

Figure 1: PL quenching on a modified MHP/TiO_2 structure (blue curve, co-doped TiO_2) with respect to the reference (green curve, doped TiO_2) (a), accompanied by TrSPV amplitude enhancement (b). In (c), a band-diagram of the DD model used to reproduce the experimental data is shown under light excitation.

[1]T. W. Gries et al., ArXiv, 2024.