Improved Hole Extraction and Band Alignment *via* Interface Modification in HTM-free Ag/Bi Double Perovskite Solar Cells

Fabian Schmitz[1], Ribhu Bhatia[2], Julian Burkhart[1], Pascal Schweitzer[1, 3], Marco Allione[4], Jaime Gallego[1], Piotr Piotrowski[5], Jakub Cajzl[5], Piotr Paszke[5], Gour Mohan Das[5], Dorota A. Pawlak[5], Federico Bella[4], Derck Schlettwein[3], Francesco Lamberti[6], Simone Meloni[2], Teresa Gatti[1, 4, *]

[1]Center for Materials Research, Justus Liebig University, Giessen, German

[2]Department of Chemical and Pharmaceutical Sciences, Universit àof Ferrara, Ferrara, Italy

[3]Institute of Applied Physics, Justus Liebig University, Giessen, Germany

[4]Department of Applied Science and Technology, Politecnico di Torino, Torino, Italy

[5]Centre of Excellence ENSEMBLE3 sp. z o. o., Wólczyńska, Warsaw, Poland

[6]Department of Chemical Sciences, University of Padova, Padova, Italy

Email address:

fabian.schmitz@phys.chemie.uni-giessen.de (Fabian Schmitz), ribhu.bhatia@edu.unife.it (Ribhu Bhatia), Julian.burkhart@ap.physik.uni-giessen.de (Julian Burkhart), schweitzer@mathematik.tu-darmstadt.de (Pascal Schweitzer), marco.allione@polito.it (Marco Allione), jaime.gallego-marin@phys.chemie.uni-giessen.de (Jaime Gallego), piotr.piotrowski@ensemble3.eu (Piotr Piotrowski), jakub.cajzl@ensemble3.eu (Jakub Cajzl), piotr.paszke@ensemble3.eu (Piotr Paszke), gourmohan.das@ibbc.cnr.it (Gour Mohan Das), dorota.pawlak@ensemble3.eu (Dorota A. Pawlak), federico.bella@polito.it (Federico Bella), derck.schlettwein@ap.physik.uni-giessen.de (Derck Schlettwein), francesco.lamberti@unipd.it (Francesco Lamberti), simone.meloni@unife.it (Simone Meloni), teresa.gatti@polito.it (Teresa Gatti)

[*]Corresponding author

Abstract

In the relentless pursuit of sustainable energy solutions to power our ever-expanding array of smart devices, indoor photovoltaics (IPVs) have emerged as indispensable assets. Among the plethora of materials vying for attention, $Cs_2AgBiBr_6$, the double perovskite (DP), shines brightly for its exceptional characteristics: ease of processing, minimal toxicity, and remarkable stability, all tailored to meet the rigorous demands of IPV applications. In this poster, we present a hole transport material (HTM)-free $Cs_2AgBiBr_6$-based solar cells, wherein the surface of the DP is subjected to a n-butylammonium post-treatment, fostering a 2D/3D mixed interface. Concurrently, the conventional metal electrode and HTM components are replaced by a carbon black back electrode (CBE) derived from upcycled biowaste. This transformative modification of the 2D/3D interface not only mitigates charge recombination but also enhances band alignment at the perovskite/CBE interface. Furthermore, density functional theory (DFT) calculations elucidate that increasing the thickness of the 2D modification augments the likelihood of hole localization near the perovskite/CBE

interface, thereby facilitating their efficient extraction. Consequently, we obtain HTM-free solar cells with elevated power conversion efficiency, underscoring the efficacy of our low-cost, end-of-waste fabrication strategy.

Keywords

Silver-bismuth Double Perovskites, HTM-free Perovskite Solar Cells, Lead-free Perovskite Solar Cells, Carbon-based Perovskite Solar Cells, Interfacial Engineering