Study of electronic properties of perovskite materials and their interfaces with extracting layers in lateral heterojunction configuration

S. Dunfield[1,2,3], **Aleksandra Bojar**[4,6,7], S. Cacovich[4,5], M. Frégnaux[8], T. Klein[1], R. Bramante[1], F. Zhang[1], D. Regaldo[4,5], J.-B. Puel[4,9], G. Teeter[1], J. M. Luther [1], M. Bouttemy[8], D. Nordlund[10], K. Zhu[1], D. T. Moore[1], M. F.A.M. van Hest[1], J.-P. Kleider[4,5,6,7], J. J. Berry[1], P. Schulz[4,5]

[1]National Renewable Energy Laboratory, Golden, CO 80401 [2]Renewable and Sustainable Energy Institute, University of Colorado Boulder, Boulder, CO 80309 [3]Materials Science & Engineering Program, University of Colorado Boulder, Boulder, CO 80309 [4]IPVF, Institut Photovoltaïque d'Ile-de-France, 18, Boulevard Thomas Gobert, 91120 Palaiseau France [5]CNRS, École Polytechnique, IPVF, UMR 9006, 18, Boulevard Thomas Gobert, 91120 Palaiseau, France [6]Université Paris-Saclay, CentraleSupélec, CNRS, Laboratoire de Génie Electrique et Electronique de Paris, 91192, Gif-sur-Yvette, France, [7] Sorbonne Université, CNRS, Laboratoire de Génie Electrique et Electronique de Paris, 75252, Paris, France [8]Université Paris-Saclay, UVSQ, CNRS, UMR 8180, Institut Lavoisier de Versailles, 78000, Versailles, France [9]EDF R&D, 18, Boulevard Thomas Gobert, 91120 Palaiseau, France [10]SLAC National Accelerator Laboratory, 2575 Sand Hill Rd, Menlo Park, CA 94205

Starting modestly at 3.8% [1] more than 10 years ago, perovskite solar cells boost the efficiencies that now approaches 25% [2], which clearly indicates that the progress in performance is occurring much faster than our actual comprehension of this material system. Especially, insight into the role that selective contacts and interfaces play under operation in the presence of mobile defects in the perovskite absorber are lacking. Hence, there is an urging need to improve our understanding of the working principle of perovskite solar cells, as insufficient fundamental knowledge of the device operation is a limiting factor in the future to further improve the performance.

It has been well documented in previous reports that optoelectronic properties of perovskites can be altered by the substrate (or selective contact) underneath [3][4][5], however so far, we do not dispose of any conclusive picture explaining this effect. In the conventional solar cell stack, a thin perovskite layer is usually buried between charge selective layers, making it very challenging to probe its properties.

Here, we fabricated a functional lateral heterojunction device, which consists of a substrate with two laterally arranged selective contacts (TiO_x as an electron transport layer and NiO_x as a hole transport layer), onto which a continuous perovskite layer is deposited. Taking advantage of now exposed perovskite surface, we used a series of surface sensitive techniques and advanced optical characterisation techniques, such as photoemission spectroscopy, X-ray absorption spectroscopy, Kelvin force probe microscopy, and hyperspectral imaging, to measure how substrate selectivity is affecting the optoelectronic properties of the perovskite.

We find evidence suggesting that the contact selectivity is inducing a carrier concentration gradient in the perovskite layer across the junction connected to the functionality of the lateral device. Furthermore, we are able to show, that by varying selectivity of the contacts through different oxidation levels we can alter the magnitude of this gradient, which in turn influences built in potential within the sample and hence the device performance.

This study provides a baseline for tailoring the selectivity of the contact materials for enhancing performance of perovskite solar cells and opening an avenue for new device architectures including buried cells terminals.

References:

[1] Green, M., Ho-Baillie, A. & Snaith, H. The emergence of perovskite solar cells. Nature Photon 8, 506–514 (2014). https://doi.org/10.1038/nphoton.2014.134

[2] https://www.nrel.gov/pv/cell-efficiency.html

[3] E. M. Miller, Y. Zhao, C. C. Mercado, S. K. Saha, J. M. Luther, K. Zhu, V. Stevanović, C. L. Perkins, J. Van De Lagemaat, Phys. Chem. Chem. Phys. 2014, 16, 22122 https://doi.org/10.1039/C4CP03533J

[4] Olthof, S., Meerholz, K. Substrate-dependent electronic structure and film formation of MAPbI3 perovskites. Sci Rep 7, 40267 (2017). https://doi.org/10.1038/srep40267

[5] Schulz, P., Whittaker-Brooks, L. L., MacLeod, B. A., Olson, D. C., Loo, Yueh-Lin, Kahn, A. (2015). Electronic Level Alignment in Inverted Organometal Perovskite Solar Cells. Adv. Mater. Interfaces, 2: 1400532. https://doi.org/10.1002/admi.201400532