MAR15-2014-020244

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Interface Energetics in Organo-Metallic Halide Perovskite-based Photovoltaic Cells

PHILIP SCHULZ, National Renewable Energy Laboratory

In my presentation I will talk about the most recent findings on the electronic structure of methylammonium lead tri-halide ($MAPbX_3$, X=I, Br) perovskite films and their interfaces to adjacent transport layers. Intricate knowledge of the electronic alignment at the contact interfaces in perovskite solar cells is essential for the understanding of the working principle as well as improving design and thus performance of respective devices. In our studies we employ ultra-violet, X-ray and inverse photoemission spectroscopy (UPS, XPS, IPES) to directly determine valence and conduction band offsets. In this way we are able to report a direct measurement of the electronic band gap as well as ionization energy and electron affinity found for perovskite surfaces. Furthermore, our findings indicate that the electronic energy level alignment of adjacent organic hole transport layers, such as spiro-MeOTAD, can limit the maximum attainable open circuit voltage (V_{oc}) in solar cells if the highest occupied molecular orbital of the hole transport material is not well aligned to the valence band maximum of the perovskite layer. Using better suited hole transporters, like CBP, values for V_{oc} larger than 1.5 V could be achieved in the case of $MAPbBr_3$ based devices. More recently, inverted perovskite solar cells based on nickel oxide bottom anodes have been reported to yield viable power conversion efficiencies and stability. We find that the interface between the p-doped NiO surface and the $MAPbI_3$ layer on top lead to p-type perovskite filsm while the same material deposited on TiO_2 in the conventional cell geometry turns out to be n-type. A further investigation of a C_{60} layer deposited on top of p-type perovskite films reveals an ideal alignment between the lowest unoccupied molecular orbital of the organic electron transport materials and the conduction band minimum of the perovskite film underneath. These results explain why the inverted solar cell structure could achieve similar successes as the conventional structure and highlight the versatility of perovskite sub-cells in potential tandem cell architectures.