Surface Energy and Microstructure: The effect of the underlying substrate on perovskite film formation for solar cell absorbers

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Electrification of the grid requires the development of efficient and reliable thin film photovoltaics with inexpensive processing. As the efficiency of hybrid perovskite solar cells has skyrocketed, practical constraints to the developing technology have put scalability and durability into scientific focus. While development of the perovskite absorber layer has received the bulk of attention, the charge transport layers located between the absorber and the contacts also have a profound impact on device performance and stability, and stand to benefit from further engineering. The use of inorganic interfacial layers, such as metal oxides, is a potential pathway for overcoming the instability and cost limitations associated with more commonly used organic interlayers.[1][2] Further, interfacial engineering of metal oxides using molecular modifiers provides a powerful tool to tune interlayer properties, resulting in improved performance and stability.[3][4][5] Careful materials characterization is required to understand the effect of these modifiers on the metal oxides, the perovskite film deposited on top, and the device as a whole.

This work details the effect of underlying layers on the growth of methylammonium lead iodide (MAPbI$_3$), a common organic-inorganic perovskite absorber. As detailed in Figure 1, MAPbI$_3$ was deposited on bare and silanized glass and ITO (indium tin oxide, a common thin film solar cell transparent electrode), to explore how the amorphous vs. polycrystalline substrates, and their subsequent modification, affect the perovskite film properties. For silanized samples, BPTMS (bromopropyltrimethoxysilane), an organofunctional silane which produces a bromine-terminated surface, was selected as a surface modifier, as Br end-groups have previously been shown to promote good perovskite film morphology and energy alignment.[3] The film stacks were characterized with a variety of methods after each step to assess the evolution of surface energy, morphology, and composition. The film bulk, surface, and interface were probed using a combination of contact angle measurements, spectroscopic ellipsometry, and scanning electron microscopy. Notably, the absorber film morphology and ultimately the stability of the film stack are sensitive to the underlying substrate; addition of BPTMS was shown to affect both of these characteristics. Figure 2 shows SEM images of MAPbI$_3$ films deposited on glass, ITO, and silanized ITO. The grain size of the MAPbI$_3$ is notably greater when deposited on the polycrystalline ITO than on amorphous glass. Silanizing the ITO results in a reduction in grain size, producing MAPbI$_3$ films comparable to those deposited on glass. The stability and composition of these materials will be compared and discussed. This work is broadly applicable to other oxides, including but not limited to transparent conductive oxides used as window layers, and modification of glass for applications such as biomicroarrays.
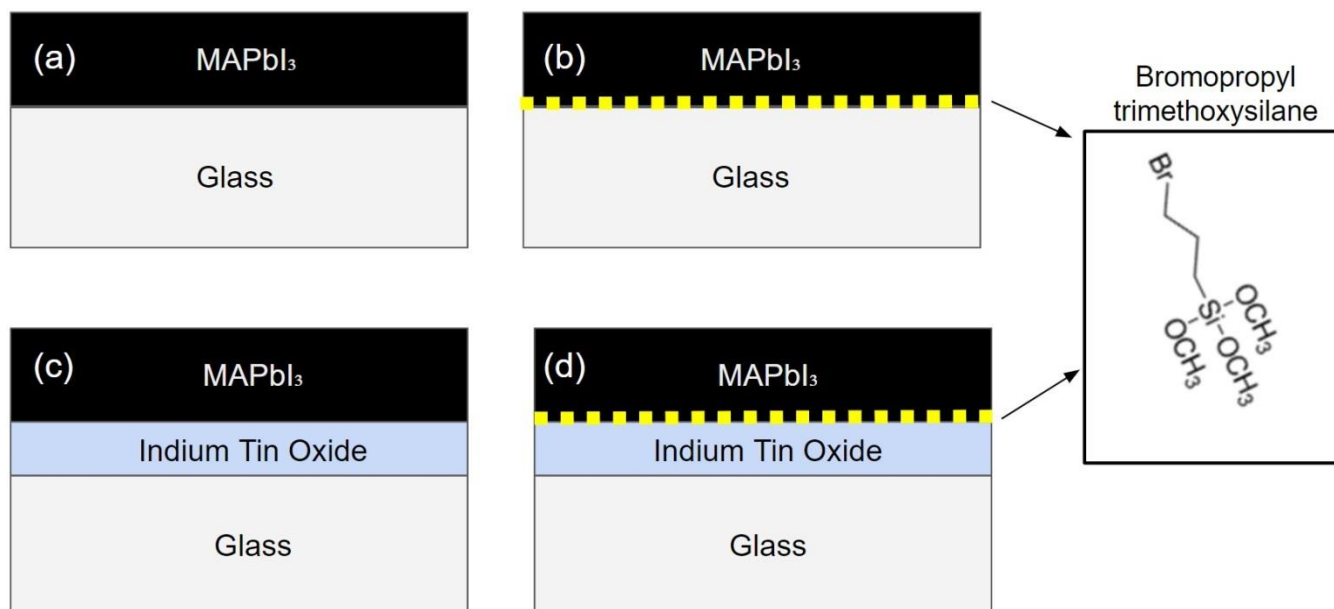
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Figure 1. Schematic of film stacks created for this study. MAPbI3 was deposited on (a) bare and (b) silanized glass, and (c) bare and (d) silanized indium tin oxide (ITO).
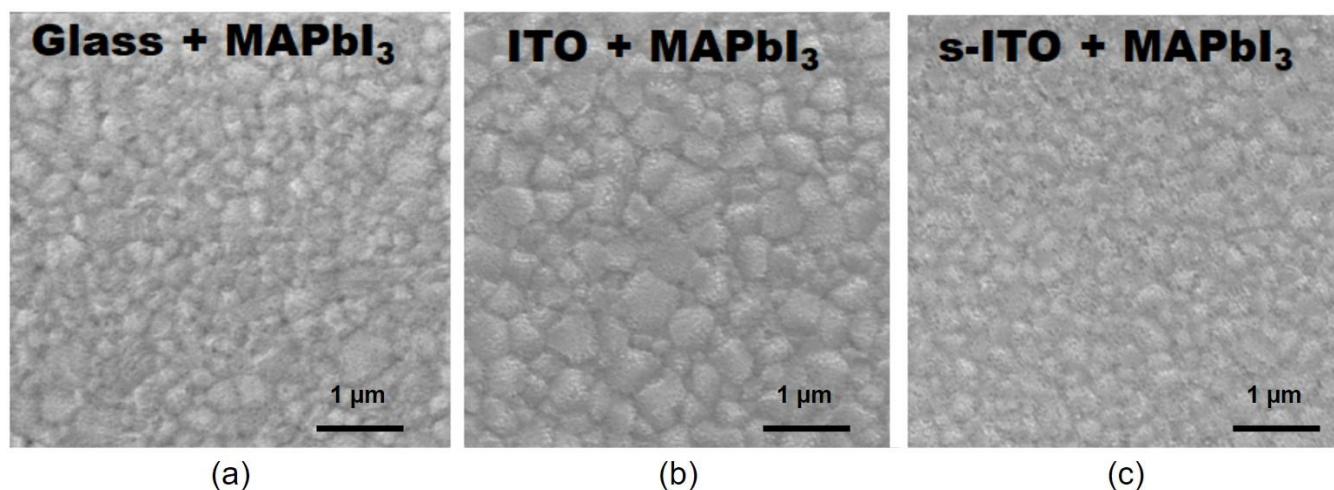

Figure 2. Scanning electron microscope images of MAPbI$_3$ deposited on (a) glass, (b) ITO, and (c) silanized ITO.

References

[1] J. A. Christians; P. Schulz; J. S. Tinkham; T. H. Schloemer; S. P. Harvey; B. J. Tremolet de Villers; A. Sellinger; J. J. Berry; J. M. Luther, "Tailored Interfaces of Unencapsulated Perovskite Solar Cells for >1,000 Hour Operational Stability." *Nature Energy* 3 (2018), 68-74. DOI: 10.1038/s41560-017-0067-y

[2] Y. Hou; X. Du; S. Scheiner; D. P. McMeekin; Z. Wang; N. Li; M. S. Killian; H. Chen; M. Richter; I. Levchuk; N. Schrenker; E. Spiecker; T. Stubhan; N. A. Luechinger; A. Hirsch; P. Schmuki; H.-P. Steinrück; R. H. Fink; M. Halik; H. J. Snaith; C. J. Brabec, "A generic interface to reduce the efficiency-stability-cost gap of perovskite solar cells." *Science* 358 (2017), 1192–1197

[3] Q. Wang; C. C. Chueh; T. Zhao; J. Cheng; M. Eslamian; W. C. H. Choy; A. K. Jen, "Effects of Self-Assembled Monolayer Modification of Nickel Oxide Nanoparticles Layer on the Performance and Application of Inverted Perovskite Solar Cells." *ChemSusChem* 10 (2017), 3794-3803. DOI: 10.1002/cssc.201701262

[4] C.-C. Chueh; C.-Z. Li; A. K. Y. Jen, "Recent Progress and Perspective in Solution-Processed Interfacial Materials for Efficient and Stable Polymer and Organometal Perovskite Solar Cells." *Energy Environ. Sci.* 8 (2015), 1160-1189. DOI: 10.1039/c4ee03824j

[5] G. Yang; C. Wang; H. Lei; X. Zheng; P. Qin; L. Xiong; X. Zhao; Y. Yan; G. Fang, "Interface engineering in planar perovskite solar cells: energy level alignment, perovskite morphology control and high performance achievement" *J. Mater. Chem. A* 5 (2017), 1658 DOI: 10.1039/c6ta08783c