Perovskites; Next Star Material for Clean Energy

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Photovoltaic Technology

One of the major challenges humanity must address is to transition away from a reliance on fossil fuels for energy production to clean, renewable sources of energy. There are three major motivations which drive research in renewable energy;

- Combatting the nonlinear climate changes that are occurring as a result of global warming, resulting from the significant emission of greenhouse gasses particularly CO_2 produced by burning of fossil fuels.
- The need to find sustainable and cost effective solutions to the depletion of conventional fossil fuel sources, since the demand for fossil fuels is predicted to increase dramatically with the growth of the global population.
- The need for many nations to improve energy security, which requires them to reduce dependence on other (less stable) nations for energy.

Energy generation from sunlight (both heat and electricity) is an ideal way to replace fossil fuel sources of energy in many situations, since the sunlight it is an abundant, clean and renewable source of energy: The energy in the sunlight incident on the Earth's surface in one hour is sufficient to meet the annual global energy demands. One of the major breakthroughs in modern science, which has attracted a great research interest is in the photovoltaic (PV), which are devices that convert sunlight directly into electricity without moving parts (except electrons!), noise or emissions. According to the International Energy Authority (IEA) it is predicted that by 2050, PVs will be the largest contributor to the global renewable energy landscape.

At present the commercial PV market is dominated by PVs based on conventional semiconductors, primarily silicon. However, there are drawbacks to silicon PVs technology, namely; (i) highly purity silicon is required, which is relatively expensive to produce; (ii) very high temperatures are required to process silicon because single crystal ingots are grown from melted silicon, thus leading to high energy outlay in production and long energy payback times; (iii) by comparison with other single junction PVs, silicon requires very thick layers

(100 - 300 μm) in order to achieve optimal efficiency due to its weak light absorption for long wavelength light. Consequently they are restricted to a rigid and flat plate designs[1] making them unsuitable for use in automobiles and many buildings integration applications, where curved PVs, or flexible substrates are needed.

The basic structure of a thin film PV devices is a hole-transport layer, a light harvesting layer and an electron-transport layer, all of which are sandwiched between two electrodes. The difference in work function between the electrodes generates a built-in electric field that facilities the extraction of photo-generated charge carriers, and at least one of the electrodes must be transparent to allow light into the device.

Perovskite photovoltaics

Perovskites are a class of inorganic materials with the general structure ABX_3 where A is an organic or an inorganic cation in oxidation state +1 or +2 (e.g.: $CH_3NH_3^+$, Cs^+, Rb^+ etc.) and B is a metal cation of oxidation state of +2 and +4 (Pb^{2+}, Sn^{2+} etc) and X is usually either a halide anion or oxygen anion (Figure 1)[2].

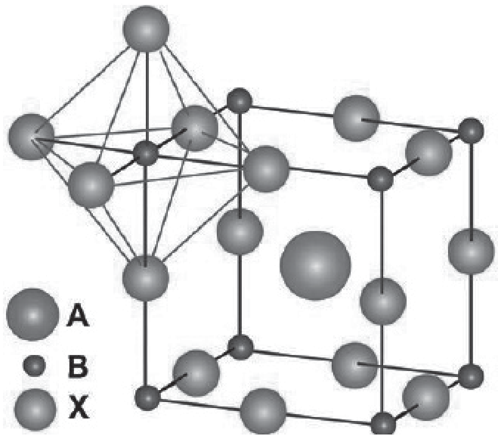

Figure 1: Crystal structure of a perovskite semiconductor with chemical formula ABX_3.

To address the drawbacks of conventional silicon PVs, perovskite photovoltaics (PPV) have begun to emerged.[3] PPV devices using lead (Pb) halide perovskite as the light harvesting semiconductor have shown an unprecedented evolution over the span of less than a decade, with the power conversion efficiency increasing from 3.8% in 2009[4] to 25.2% in 2019[5]. The ease of synthesis of perovskites is a key reason for the rapid and intensive research interest in this area. Lead halide perovskites are also compatible with lightweight flexible substrates[6] because they can be processed from solution at low temperature[7], which ensures a greatly reduced energy outlay in production in comparison to conventional silicon solar cells, and are amenable to facile tuneability of the absorption spectrum via halide mixing/exchange, which is important for applications where the aesthetics are important such as buildings integration applications[8]. Most importantly PPVs offer a potentially very low carbon footprint in production as a result of the low processing temperature and potential for fast roll-to-roll manufacturing, so they can return the energy used in their production within a few months of installation, much less than the 1 year energy payback time of conventional silicon PVs[9].

PPV device architecture and operating principles

The typical structure of a PPV device consists of a light harvesting semiconducting layer sandwiched between electron and hole transporting materials (Figure 2). The charge transporting layers are chosen to ensure optimal alignment of the electrode Fermi levels with the relevant band edges in the light harvesting semiconductor.

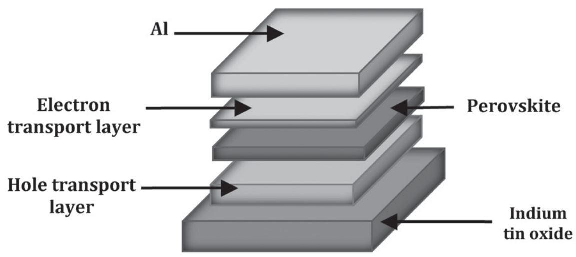

Figure 2: Simplified device architecture of a general perovskite PV device

Initially light passes through the transparent, wide band gap metal oxide electrode; usually Indium tin oxide (ITO). The light harvesting material absorbs photons of light with energy equal to or greater than the band gap via the excitation of electrons from the valence band into the conduction band. Due to the relatively large dielectric constant in perovskite semiconductors the photo-generated electron and hole are not coulombically bound to one another at room temperature. These free charge carries are selectively extracted by an electron transport layer (ETL) and a hole transport layer (HTL) respectively. The separated charge carriers move from their respective transport layers to Fermi level (Ef) of the respective electrodes from which they can flow into the external circuit.

When the two materials in the PPV device come into contact, charge transfer will occur causing an alignment of the Ef, as the electrons will move from higher lying Ef to the material with the lower lying Ef. The equilibration of the Efs of the perovskite and the metal results in formation of a depletion region (W) where all of the transferred charge is concentrated. This charge transfer causes a VL shift at the interface forming a Schottky barrier.[10] (Figure 3).

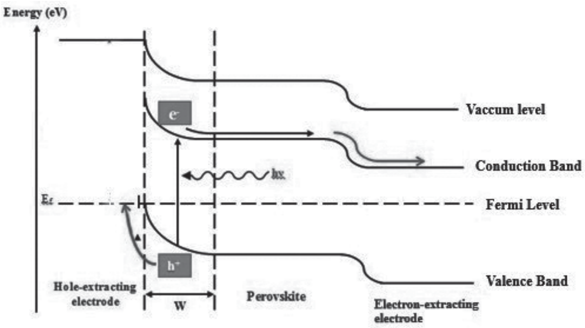

Figure 3: Band diagram for the operation of a Schottky PV device.

The disadvantage of lead halide perovskites for utility in PV devices is the possibility of lead contamination of the environment due to failure of the device encapsulants or improper disposal at the end of life, which is a barrier to commercial exploitation in many parts of the world.[11] This is because lead is well-known to be a highly toxic element that accumulates in the food chain[12] and lead halide perovskites readily decompose upon exposure to moisture and water to form lead compounds with significant solubility in water.[13] Consequently, there is great interest in the development of lead-free alternatives matched to the needs of PV applications.

References

1. L. Yalçin and R. Öztürk, J. Optoelectron. Adv. Mater., 2013, 15, 326–334.
2. X. Zhao and N. Park, 2015.
3. A. Mei, X. Li, L. Liu, Z. Ku, T. Liu, Y. Rong, M. Xu, M. Hu, J. Chen, Y. Yang, M. Grätzel, and H. Han, Science, 2014, 345, 295–298.
4. A. Kojima, K. Teshima, Y. Shirai and T. Miyasaka, J. Am. Chem. Soc., 2009, 131, 6050–6051.
5. Best Research-Cell Efficiency Chart | Photovoltaic Research | NREL, https://www.nrel.gov/pv/cell-efficiency.html, (accessed 05 December 2019).
6. M. Kaltenbrunner, M. S. White, E. D. Głowacki, T. Sekitani, T. Someya, N. S. Sariciftci and S. Bauer, Nat. Commun., , DOI:10.1038/ncomms1772.
7. K. S. Chen, H. L. Yip, J. F. Salinas, Y. X. Xu, C. C. Chueh and A. K. Y. Jen, Adv. Mater., 2014, 26, 3349–3354.
8. L. Yalçin and R. Öztürk, J. Optoelectron. Adv. Mater., 2013, 15, 326–334.
9. M. J. Griffith, N. A. Cooling, B. Vaughan, D. C. Elkington, A. S. Hart, A. G. Lyons, S. Quereshi, W. J. Belcher and P. C. Dastoor, IEEE J. Sel. Top. Quantum Electron., , DOI:10.1109/JSTQE.2015.2487968.
10. K. P. Marshall, M. Walker, R. I. Walton, and R. A. Hatton, Nat. Energy, 2016, 1, 1–9.
11. F. Giustino and H. J. Snaith, ACS Energy Lett., 2016, 1, 1233–1240.
12. A. Babayigit, A. Ethirajan, M. Muller and B. Conings, Nat. Mater., 2016, 15, 247–251.
13. G. Niu, W. Li, F. Meng, L. Wang, H. Dong and Y. Qiu, J. Mater. Chem. A, 2014, 2, 705–710.