

The “Levelized” cost of electricity and perovskite photovoltaics.

W. Nie et al., Science 347, 522–525 (2015).

D. Shi et al., Science 347, 519–522 (2015).

de Quilletes et al. Science 348, 683-685 (2015)

W. Tress et al. Energy Environ. Sci. 8, 995-1004 (2015)

Recommended with a Commentary by Albert Migliori, Los Alamos National Laboratory

The big three of grid-scale renewable energy sources, excluding hydroelectric power, are photovoltaics (PV), wind, and concentrated solar thermal (mirrors and steam turbines). Because each of these sources of clean energy is widely used on utility grids today, they are more or less economically competitive. This is an essential point as the economic bottom line is, in the end, all that matters to utility operators. Thus the race to drive down cost is the driver for basic research into PV materials because only PVs require a deep understanding of condensed matter physics.

In implementing a PV array, there are two essential components. They are the electronics to convert the DC produced by the array to the AC needed by the grid, the (inert) supporting structures and land to mount the PV materials on, and the PV material itself. Everything but the PV material is dubbed the balance of system (BOS). For implementations of PV systems, the cost is about the same for such things as maintenance of generating facilities required to back up PV when it cannot be dispatched (no sun), capacity factor (how much of the time does the capital investment produce) and more. These are irreducible components of the BOS which in turn is a major component of the “levelized” cost of electricity (LCOE), a somewhat ambiguous measure of the value of an electrical generation capability. The LCOE, including capital costs, operating costs, fuel costs, and more is an attempt to measure the present monetary value of the total cost of a generating facility over its full lifetime against the total electrical energy ever generated by the facility. The units are e.g. \$/joule. The scientific issues for the LCOE are tied to cost per watt (\$/W) to make a PV cell, and efficiency because low efficiency requires more land and supporting structure, increasing the BOS cost, and lifetime of the facility. And, rightly so, current scientific interest lies in addressing, more or less, these three critical factors, but not explicitly. Let’s take a look at these factors, and how they are, or should be, driving recent PV research.

Most PV cells are semiconductor diodes, a sandwich of p-type (holes are the majority charge carrier) and n-type (electrons are the majority carrier) semiconductors. When a photon penetrates a PV cell, it generates an electron and a hole. The diode has an intrinsic electric field between n- and p-type semiconductors forming what’s called a depletion region with a high electric field

driven by the chemical potential difference between the two types of semiconductors. The electric field sweeps the hole one way and the electron the other. If they make it to the surface of the cell, a very substantial charge difference builds. Connecting one side of the cell to the other through an external circuit provides a path for the charge imbalance to correct itself, and in the process, produces electrical energy in the connecting circuit.

Today, most grid-scale (but not all) PV materials are made from single crystals of Si. Because crystals are so perfect, there are very few defects and traps for the photo-generated electrons and holes, and so most make it to the corresponding electrodes for collection. Thus defects of various sorts play an essential role in degrading the efficiency of a PV cell. But the huge single crystals needed for high-efficiency Si PV cells are extremely demanding to produce. They must be grown from exceptional-purity molten Si slowly and carefully, then sliced into wafers. And that's just the starting material.

If one could make an efficient PV material directly on a substrate from a solution of chemicals, such a process would be very interesting and that is exactly how a perovskite photovoltaic (PPV) cell is made using organo-lead trihalide MAPbX_3 ($\text{MA} = \text{CH}_3\text{NH}_3^+$; $\text{X} = \text{Br}^-$ or I^-) perovskites. They are basically produced using wet chemistry so that the $\$/\text{W}$ is intrinsically low. However, just like Si, PPV must have a low defect density and large crystalline grains to be efficient, necessary to keep the BOS costs low.

Two recent back to back articles in *Science* [Nie, Shi] address more or less directly $\$/\text{W}$ and indirectly via efficiency, BOS. Nie discusses solution-chemistry approaches to making PPV that show remarkable large grains with excellent electron-hole transport dynamics indicating few defects and traps, while Shi describes the production of very large single crystals of PPV. The primary focus is photoluminescent decay times (PLD) and carrier lifetime, studies of which are exemplified by [de Quilletes]. PLD is extremely important because a long PLD means that electron-hole pairs can't find useless decay modes at defect and trap sites and so resort to recombination via exactly the effect that generated them in the first place. That gives the system lots of time to collect the carriers on electrodes and deliver them to an external circuit, generating electricity. There are other decay mechanisms that destroy photo-induced carriers without generating electricity. These mechanisms catch carriers before the electrodes can, also affecting efficiency. In both cases, it is known from 75 years of semiconductor research that crystallographic defects, grain boundaries, impurities all make things worse. Thus it is important to make the best PPV crystals possible, either in films or bulk. Unfortunately, the two fabrication papers [Nie, Shi] show results that very weakly connect what they did to general principles that might direct future work in that basically they just tried stuff to see what would happen; both obtained good results, but where does one go from here? Nevertheless, they are defining example processes that did improve the efficiency, and lay the groundwork, for estimating the costs to produce cells that

are at best 20% efficient. This compares to the 24% efficiency of single-crystal Si PV. That 4% (which is 20% lower than Si) is critical because it drives the BOS. The BOS includes the frames, supports, land area, electronics, and more needed to go from a laboratory cell to a generating plant. If PPV are 20% less efficient than the now under \$0.68/W, down from many dollars/W a few years ago, Si cells, then PPV require 20% more structures and land to generate the same power. With very low Si costs, the BOS becomes a very much larger component of the LCOE, and the cost of making PV cells is correspondingly a smaller component. Thus the importance of cheap PV cells is a lot lower than it was recently, and so one real driver now is efficiency because it reduces BOS.

In the work by [de Quilettes] some real approaches to improving efficiency are revealed in their detailed measurements of grain-by-grain PLD. They observe “dark” grains with short PLD and “bright” grains with long PLD. This is an enormously important clue for the PPV material fabricators. If it can be sorted out exactly what effects make grains dark (and right now only conjectures are flying), then that may be able to direct fabrication to eliminating them. In numbers, perhaps 30% of the grains are dark. Eliminating them would improve efficiency by more than 30%, reduce needed collector area, and so drive the BOS cost to below that of Si.

There is another issue. The efficiency measurements are sketchy because there are mysterious hysteresis effects and degradation effects that are not yet understood. That is, the measured efficiency depends on how and when the measurement is made, with efficiency changing a lot depending on the illumination time and the direction of voltage sweeps during the measurement. In the work by [Tress] some real science is being brought into this effect, relating it to space charge buildup at the electrodes from loose carriers, much like the Debye screening layer in electrochemistry, thereby reducing the electric field that separates electrons from holes for collection at the electrodes. This may point the way for the material fabricators.

Finally, all the PPV materials are water sensitive, likely UV sensitive, and so require exceptional environmental protection, unlike Si. Right now, degradation time scales are days or weeks, making them unsuitable for utility-scale power generation. Short PPV lifetimes greatly increase the LCOE because the lifetime of the facility is shortened, or, at best, the replacement interval for panels increases maintenance costs. This is a critical area to be addressed, and the field knows it.