

Perovskites

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Abstract

Silicon Based Semiconductors are currently the most reliable type of Photovoltaic Solar Panels on the market (8). This paper covers the fastest growing and biggest competition to this material in Perovskites, a lattice structure consisting of a 3-level lattice-crystal that with many undiscovered modifications that leave room for endless improvement. This paper collects and presents key research that is being performed on such models with an emphasis on efficiency and reliability. This paper will effectively demonstrate why investors and businesses should put their money where their logic is and expand this industry for the better of the world's energy-related future all the while informing readers on the potential downsides to such models through potential risks and fundamental fl

INTRODUCTION

Perhaps you visited the gas station lately and filled your tank so that you could transport yourself to your job, your house, or even your grocery store. It is quite possible that you did not realize that you just contributed to taking up a limited, valuable resource of our planet. This is not to put shame on you as everyone is liable and exposed to using this and other natural resources on earth, but it is important to understand that these resources are, to the scientific community's knowledge, limited. They will eventually run out neglecting a conservation program so it up to the generations of tomorrow to find alternative sources of energy for this problem. Perhaps the biggest and fast-growing sources of energy with the most potential is solar energy. Solar energy is the concept of collecting sunlight from a stationary device in converting that collected sunlight into electricity which can be used to power essentially anything (9). Such a technology is not as simple as the combustion-dependent natural fuels of the earth, but it relies on something that is clear as day: the sun (9). This technology is not the current go-to option for energy as the not enough progress has been made in the field of renewable energy to overtake the easy option of natural fuels (9). But with continued efforts and focus towards such as subject, as has been the case for most every technology in the history of man-kind, results will come. Results of this research are intended to convince many investors to shift their money towards this business and invest in such a manner that demand for said products increase which in-turn will increase the demand for said research.

With such a large implication on the future, clarification and specification are important to portray an accurate depiction of the economy's next driving force. The focus of this paper will be perovskite solar panels. The two main facets of perovskites that will be analyzed are efficiency and reliability. Potential sub-topics include the pricing but for the simplicity of this paper, economics of potential models will not be analyzed as there are dependent on a large variety of unrelated factors. This presentation aims to clarify potential solutions towards improvement of these facets, composed of an in-detail summary and relevant contextualization. Many concepts will be presented are to be digested for this paper to adequately interpreted. Solar panels reside in locations that include rooftops and fields, settings that contain no visual interference on an upward 180-degree sphere with respect to the surface (9). PV systems convert sunlight into energy that can be used for custom limited purposes, whether that be residential or industrial. Residential

settings are more of a current destination for such technologies as the reliability of these up-to-date models are not trustworthy enough for an industrial setting in which much more than a refrigerator cooling is at stake. Solar perovskites models currently have efficiencies that range around the mid-20's (8). Historical trends can be demonstrated below in figure 1 courtesy of the National Renewable Energy Laboratory, an institution that is required to test and verify any efficiencies that aimed to be published in research journals (8). This illustration shows perovskite models (red) vs every other notable PV model. This graph depicts the unparalleled acceleration in performance compared to other models.

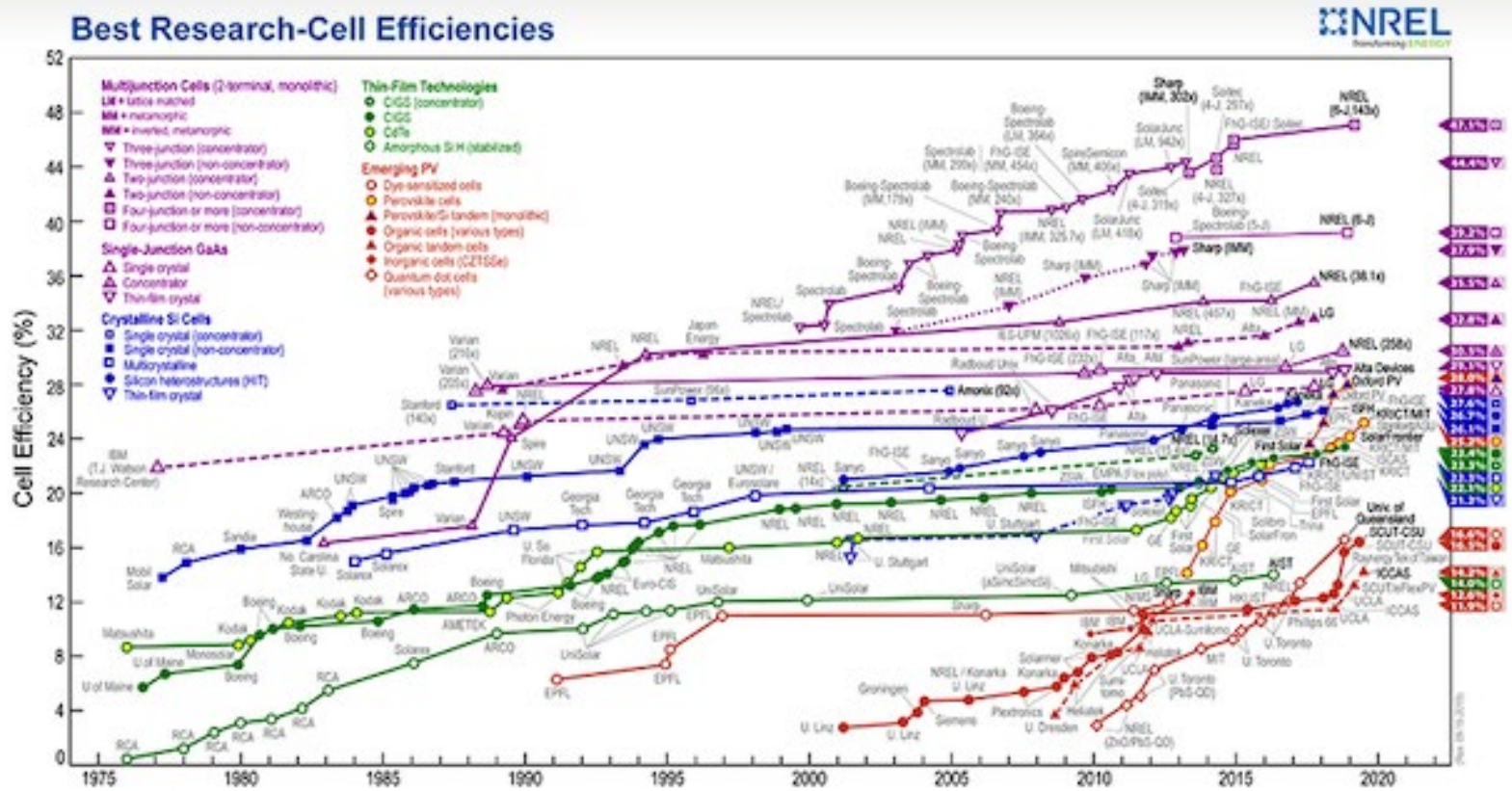


Figure 01: NREL Efficiency data of different Solar PV Models throughout years (8)

STRUCTURE

To interpret the advancements and milestones that are being reached for perovskite models towards efficiency and reliability, it is crucial to have a basic understanding of perovskite solar system structures. Structures are known to fluctuate to a degree both in pure perovskite models and in hybrid perovskite models. Pure perovskite solar cells are known to contain purely inorganic materials, while hybrid as assumed contain a mixture of inorganic and organic materials (3). Organic Materials in this context are known to produce higher efficiencies but less reliability while Inorganic materials typically withhold higher reliability (3). Certain hybrid-compositions have led to a shift in research in recent years in favor of such models that attempt to find an optimal compromise. These

materials, organic and inorganic, compose of the perovskite layer in a solar panel (3). There are of course other layers that should be mentioned before further discussion of these composition and their properties are reached. The two main structures that apply to most perovskite cells of interest are mesoporous (mesoscopic) and planar heterostructure (which is often just denoted as planar) (3). The only considerable difference between these two is the mesoporous oxide layer that resides around the perovskite layers of mesoporous structures (3). Planar heterostructures on the other hand do not have this oxide layer which serves as a purposeful technique of absorbing more sunlight within the respective perovskite layer(3). Outside of the perovskite layer for both mentioned structures, metal electrodes, hole-transmitting material (HTM), and electron transport materials (ETM), and fluorine-dope tin oxide glass (FTO) are observed to compose the structure of these two models which are illustrated in figure 2) in addition with exterior glass and other supporting materials (3)(5). The second figure is being

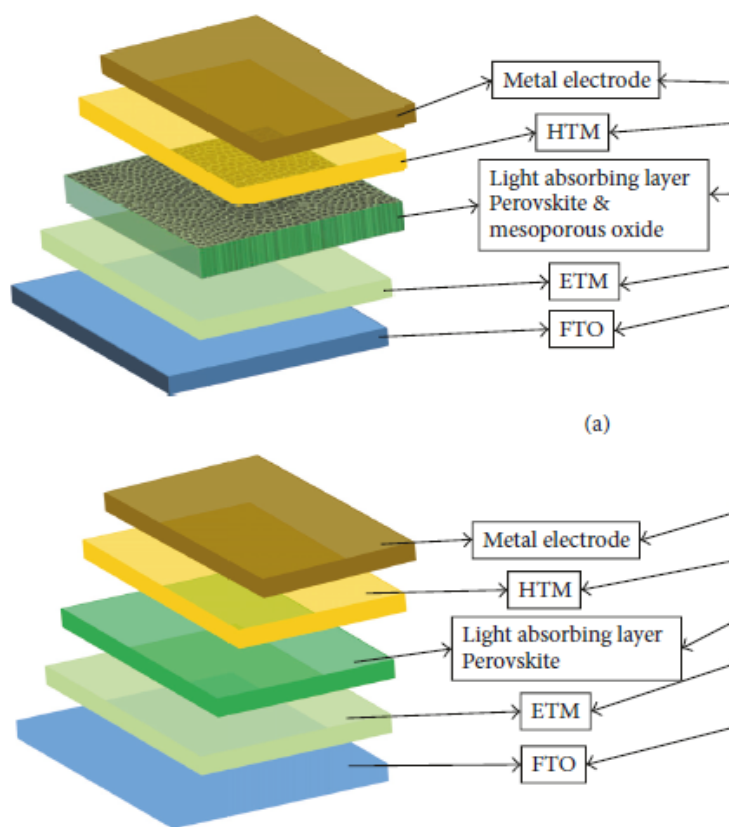


Figure 02: PV layer visualization with mesoporous (top) and planar heterostructure (bottom) (3)

referred to upside down with respect to the sun, meaning that sunlight first contacts the FTO layer (3)(5). FTO's are the most used bottom

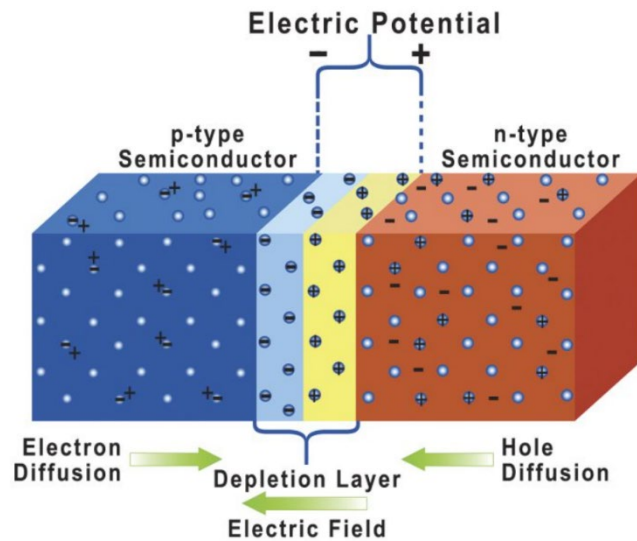


Figure 03: Different layers (junctions) with respective holes and electrons (16)

electrode layer for modern day perovskite-based solar panels (3). This is one of the two electrodes in a typical solar panel that allows (3)(5). The electrodes, that being the metal electrode and the FTO in this context, are technologies that reflect moving electrons attempting to escape back into the core of the system (3)(5). The metal electrodes reside on the opposite side of the structure with respect to the sun and are often classified as anions or cations depending on the interchangeable structure that can be designed by swapping the ETM's and the HTM's along with their respective junctions (3). FTO's are the most expensive part of most solar panels as they are electrodes that serve two purposes: let

sunlight in and not let electrons out (5). The focus of this research will not be on this layer despite its high potential for improvement and high demand for improvement. The mid-layers of a solar panels are known in this context to be HTM's and ETM's, materials that carry holes and electrons, respectively (3). The transport of these materials is executed to create a current, as the holes have a positive charge and electrons have a negative charge (3)(6). The layer of interest is the Perovskite layer which resides in the center of these models and consists of a p-n junction, where the P-junction contains electron sufficient lattices, and the N-junction contains electron deficient lattices (3) (6). Such difference is critical when the sunlight enters the systems and contacts the P-junction, where sufficient energy eject electrons from this lattice and towards the ETM which is paired with the P-junction (3)(6). This symmetrical relationship predictably yields an N-junction that is paired with the HTM, which despite its name completes a circuit for the electrons flowing in the ETM and delivers them to the holes residing at the edge of the N-junction, where they fulfill the charges (3)(6). It takes enough sunlight to create a potential energy difference so that the flow of electrons and holes occur in their respective regions (3). This flow of electrons around the P-junction to the N-junction can be demonstrated in figure 3) and is what creates an electrical circuit for power generation (3)(6)(16).

Function

The structure of the FTO, ETM, HTM, and Metal electrode are universally recognized as the necessary and included components for most any type of Solar Photovoltaic compound with the same basic function regarding the electron/hole movement. What differentiates and defines Perovskite models is the composition of the semiconductor

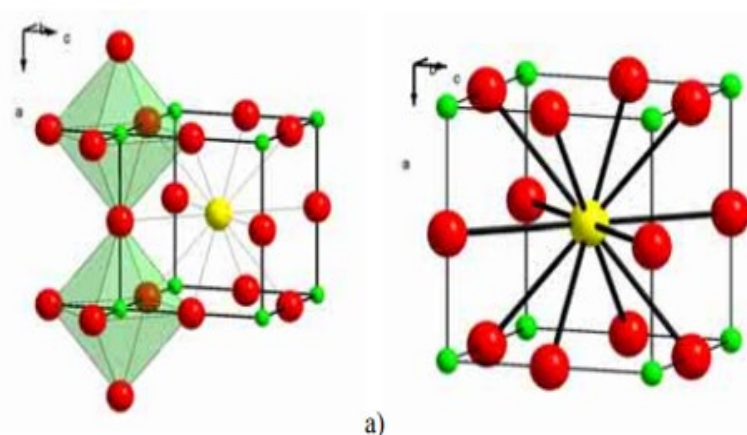


Figure 04: Crystal Lattice Structure for a typical perovskite solar cell. A-site is represent by green balls, B-site by yellow, and X-site by red (14)

material in between theses established layers (3). This research will not focus on other PV semiconductor compositions but will rather discuss the basic criteria for a perovskite semi-conductor and discuss specific perovskite compositions as they are relevant to specific advancements that will be referred to in this research. The semiconductors of perovskites are composed of a highly organized, octahedral crystal-lattice structure with 3 different molecule/atom classifications denotated as ABX_3 (3). This structure is illustrated in figure 4). The A and B components are representative of cations, with the

larger cation of the two being A (3). The A cation is most often methylammonium (MA) or formamidinium (FA), alloy molecules that are much larger in size than the B ions which is typically Pb^{2+} or Sn^{2+} (3). The X component which has a subscript of 3, indicating that it is 3 times more present in a given crystal-lattice than A or B, is a halogen anion which is most often Cl^- , Br^- , or I^- (3)(4). A is perhaps the most interesting of the 3 components, as it has the most possibilities and due to its size, the most influence on a perovskite's properties (3)(4). It is important to note that the distinct assignments of these different species to their relative position (A,B,X) should only be used as a basis for learning these concepts. In research and industrial settings, these positions/layers are subject to multiple ions/molecules with specific proportions (1)(2). For example, the B component of a perovskite crystal-lattice could theoretically consist of 20 percent Pb^{2+} and 80 percent Sn^{2+} . Functions are derived based of behavior that show that show how the change in concentration of two species relative to a particular position influences such properties as Band Gap Width (2). These anion compounds can

either be organic or inorganic, with recent research indicating that there is more performance potential with organic compounds such as MA and FA because of their mixture with inorganic metal cations (B) and halogen anions (X) (3)(4). Both MA and FA are alloys, a property that makes the crystal lattices thin, flexible, and lightweight, a trait that is denoted by the term “thin-film” (3)(4). This unique property of Perovskites is a big reason as to why research in this subject matter has boomed in the last few years due to the fact that it allows for easier transportation and installation of said technology (8).

Efficiency

There are many possible methods for improving the efficiency of a given solar panel. For simplistic and relative research, efficiency improvements towards perovskites will only be looked through the perspective of band-gap width. Band gap is the amount of energy measured in electron-volts that is required from the incoming light photons to eject the electrons

from the from their valence shells and get them to the ETM layer (11). As illustrated in figure 5, there is an optimal band gap for a given perovskite models that fluctuate accordingly as the properties of that model differ (11). Dr. McGehee, a Professor of Chemical and Biological engineering at the University of Colorado Boulder, and his research group analyzed different concentrations of A and X site molecules for a Perovskite/Si (Silicon) Tandem Solar model (2). This type of solar structure, commonly defined as a “two-terminal tandem” model, consists of two semiconductors which is easy to visualize as a double burger with the bun between the patties (2)(6). It was previously known going into this research that the

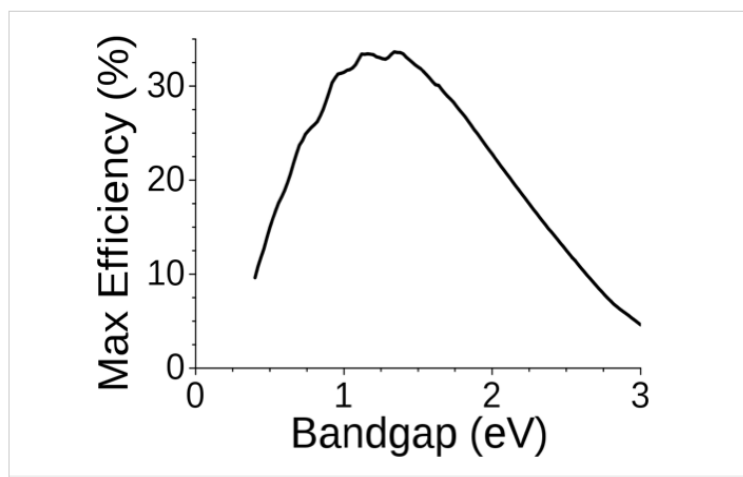


Figure 5: Optimal band gap range for a typical PV model in relation to Efficiency (11)

perovskite/Si solar cell performs best with a precise band gap of 1.67 eV (2). Three halides were to be implemented into this model, those being Chlorine, Bromine, and Iodine (2)(5). The first step of this research was to determine the Cs composition that was to be paired with FA for the organic alloy in the A site in the double-halide perovskite $\text{Cs}_{1-x}\text{FA}_x\text{Pb}(\text{I}_x\text{Br}_{1-x})$. Cs was determined to have a composition of 25 percent (2). They originally determined that it was the better alternative to its lower counterpart of 17-percent Cs due to its aligned properties in reliability

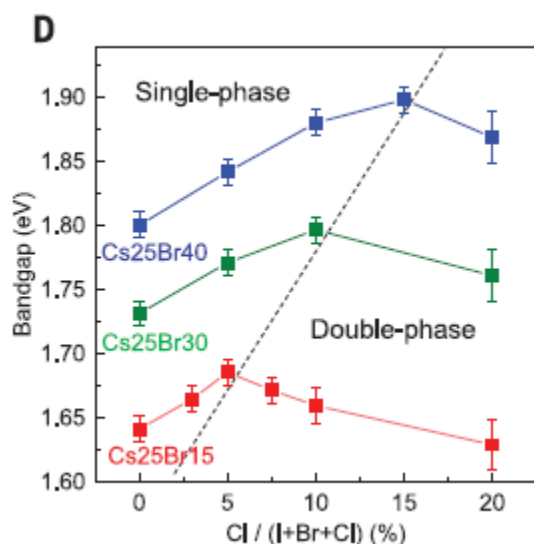


Figure 06: The 3 different models of Bromide concentration that were tested to find the optimal band gap (1.67 eV) (2)

responding to sunlight-induced wavelength and resultant voltage produced. This produced a 1.63eV band gap so from there it was necessary to combine this type of double-halide in solution with MAPb(Cl₃), molar concentrations 2 and 5 percent, to reach the desired band gap of 1.67eV (2). While the relative Cs concentration of the double-halide was determined, the bromide concentration relative to Iodine in the X-site still needed to be confirmed through an experiment (2). For future reference, the combination of the double-halide and single halides in solution that are mentioned above will be referred to a triple-halide for simplistic purposes. It was found by analyzing the inflection points of different concentrated models that the lower the bromide the concentration, that is around 15 percent, the closer the produced bandgap was to the desired value (2). These triple halides, subject to several advanced methods, eventually produced a 30 percent relative increase

in efficiency in the given model two-terminal tandem from 21 percent to 27 percent (2). It is evident that the modification of such minor perovskite properties have major implications on the overall efficiency of a model.

Reliability

It was referred to in the first research that while the main component of a solar panels is the semiconductors and they and their properties have the most implication not only on the efficiency of a model but also the reliability (9). Perhaps outside of the semiconductor layer itself, the layers that interact with the semiconductor material are a stand-alone second with respect to efficiency and reliability implications. These will be referred to as monolayers and are not to be confused with the previously mentioned mesoporous layers mentioned in the structure section of this research. In the referred to research conducted by Zhenghong Dai (Ph.D. candidate) and company at Brown University's engineering department, a well-known Ivy League school (1). The paper was published by the American Association for the Advancement of Science Journal very recently (5/2021) (1). Dai and co. discovered through their findings that adding an Iodine-terminated self-assembled monolayer (I-SAM) increased the 80 percent efficiency retention time from 700 to 4000

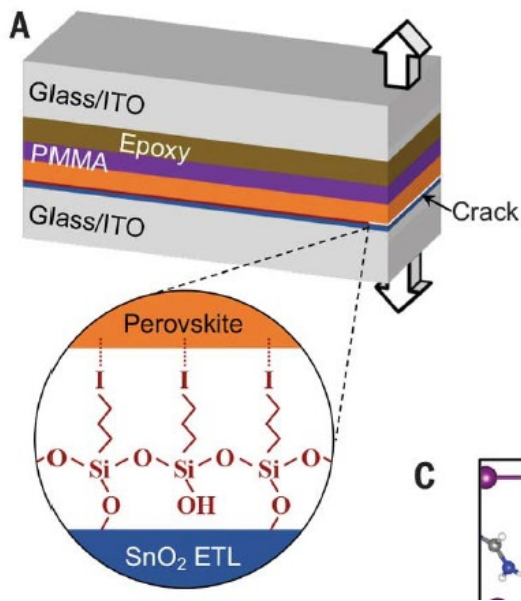


Figure 07: The molecular composition of I-SAM layer injected between the semiconductor material and the ETM (1)

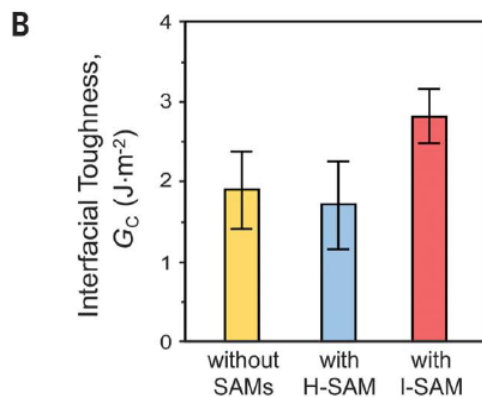


Figure 08: Reliability performance of specific layers (1)

hours of operation (1). The layer was installed to sit between the ETL (electron transport layer, same as ETM) and the perovskite semiconductor material which were described to be metal halide perovskites (MHP) with a composition of $\text{Cs}_{0.05}(\text{FA}_{0.85}\text{MA}_{0.15})_{0.95}\text{Pb}(\text{I}_{0.85}\text{Br}_{0.15})_3$ with 4% mole excess PbI_2 and SnO_2 (1). The I-SAM, that is the monolayer that was installed, consisted of 3-iodopropyl trimethoxy silane ($\text{Si}(\text{OCH}_3)_3(\text{CH}_2)_3\text{I}$) because of its unique ability to not only bond to the ETL oxides of SnO_2 but form horizontal (with respect to layers), cross-linked chains shown in figure 7 (1). The -I terminal group at the end of the alkyl chain groups form bonds with the MHP thin film groups to complete the structure. The lyophilic, compressed structure of these chains reduces the electrostatic tension between the ETL and the MHP allowing for a much smoother, improved transportation process of electrons between the two surrounding layers (1). This behavior in the long run prevents damage on the system to a significant extent which is measured through the toughness coefficient G_c in Joules/meters² that is illustrated in figure 8 (1). This research performed was relatively new and it cites how there has not been much research in this direction that they are aware of (1). They are basically implying these interconnecting I-SAM monolayers will be investigated a lot further in the future and that significant advancements will be made towards improving the reliability of perovskite solar models.

Stakeholders and Issues

Such technology obviously has significant implications on the energy consumption of the future.

As a result, there is a growing demographic of stakeholders to this issue and for a variety of reasons. Many stakeholders are seeing the cost of such technology decrease in an inversely proportionate relationship to the amount of research being conducted towards this subject (13). Much to the parallel of electric cars, this technology can supersede natural gas and fossil fuels once the cost is in a completely feasible range. It also helps that such an investment rids the annoying monthly fee of electricity to a prominent extent if an adequate

amount of this technology is installed. At this point, the only reasonable speculation against investing such technology is the rapid appreciation in performance that is occurring. This phenomenon is demonstrating in figure two, and with the exponential growth in this field one can expect performance to skyrocket once the major, expected breakthroughs come (8). From this appreciation, it can be reasonably expected that rebate/trade-in programs will be incentivized to encourage consumers to invest in the latest models without worrying about the model getting outdated within the incoming years. Another considerable interest of potential investors is the typical profit margins and the recent trends related to such issues. Businesses models have the current profit margins at 6 percent, mentioning that long term investments are required for this profit margin to exceed that average, but this is the case with most profitable businesses (12). The promising aspect is that the same source cited that solar panel industry is growing about 15 percent annually in large city markets, indicating that such a start-up should take place in a heavy populated area (12).

CONCLUSION

Perovskites Solar Panels are a technology in which the future remains largely uncertain. This is due in massive part to the rapid acceleration of advancements pertaining to this device in recent years. Perovskite solar cells produce efficiencies of around 3 percent in 2006 and has since grown to a staggering 25 percent (8). There has been much speculation as to whether this number will plateau in the upcoming years and reasonably so. Like any research towards a new technology, there is no absolute certainty as to whether the technology will significantly improve. But this thought process has always been continued throughout human existence and it mostly stems from complacency and overreaction to the latest and greatest of a given model. Take the smartphone for example which emerged in the late 2000's. Most everyone was so perplexed by the idea that a computer could be simplified and compacted into a phone that they lost track of what could be done. Civilization was so caught up in what was happening in the now that they lost sight of what would and could occur in the future. Technology is much paralleled to human civilization in the fact that it evolves and changes in large part to our adaptation towards what needs to be accomplished. As long as research organizations remain open-minded and focused about the possibilities pertaining to this subject, the possibilities will remain limitless. With this being said, Solar panels are the technology of the future which have an undeniable demand due to the growing issue of limited natural resources such as natural gases and

fossil fuels. It is only a matter of time before this technology is a commodity and not viewed as the next big thing of the future.

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