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What does net zero by 2050 mean to the solar energy materials researcher?

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The energy sector is today the largest greenhouse gas emitter, accounting for $\sim\!\!70\%$ of anthropogenic CO₂ emissions. Rigorous decarbonization of the global energy supply is required to limit the temperature rise to below 1.5°C and reach net zero by 2050. Solar photovoltaics will play a key role, and massive upscaling of solar photovoltaics is faced with many challenges. Here we discuss how materials researchers can contribute to this global grand challenge.

Harvesting earth's most abundant renewable energy source—the sun's energy reaching the earth—using solar photovoltaics (PV) (Figure 1A) will play a key role in decarbonizing electricity production. Solar energy is the renewable source capable of scaling to the tens of terawatts on which humankind will rely.

The importance of PV to net zero targets is seen in its projected contribution to world electricity capacity, which has only increased with progressive iterations of the International Energy Agency (IEA) reports (Figure 1B, inset). To meet our collective net zero goal, massive scaling of solar PV is required (Figure 1B): the boldest scenario described by the International Technology Roadmap for Photovoltaics (ITRPV) envisions a world in 2050 powered 100% by renewable energy, with solar PV contributing to 69% (versus 1% in 2020) of the global energy supply, including power, heat, and transport.²

Upscaling PV deployment from gigawatt to terawatt capacity comes with significant challenges. 2020 set a record for the annual increase in PV generation of 156 TWh (23%); yet this figure lies below the 24% growth target set by

even the *least* aggressive IEA net zero scenario.³ Analysis suggests that it may be hard to maintain a high growth rate while keeping profitability. Expansion of PV manufacturing requires new factory capital expenditure, which increases the PV module minimum sustainable price. In the case of technologies that are capital intensive, this curtails the potential for growth range in annual PV manufacturing capacity, in some cases to roughly 20%.^{4,5},

Ultimately, the levelized cost of electricity (LCOE, measured in \$/kWh) will influence PV's competitiveness in the electricity market. It will impact success in displacing fossil fuels. Over the past 15 years, cost advantages associated with crystalline silicon (c-Si) PV scale up have driven a steady drop in prices. For every doubling in the cumulative installed capacity, the price per watt has dropped by 40%.² Signs of diminishing returns in Si are showing: the manufacture of c-Si PV panels is now far down the learning curve, ensuring that additional costs such as those of inverters and land acquisition are of increased overall prominence. To extrapolate from the experience of mature PV markets such as Germany, high growth rates in PV capacity are likely to slow once the largest markets

(China, India) reach a critical installed capacity. Beyond this critical number, new installations produce diminishing returns because grids are not yet fully equipped to store nor to manage time-varying production. Avoiding the PV plateau is not the concern of PV researchers alone; it requires action on three fronts: (1) innovations in PV technology that can cause a step-change in the LCOE, (2) next-generation grids that manage time-varying production with storage, and (3) electrifying heating, cooling, and transport, which make up the lion's share of energy usage.

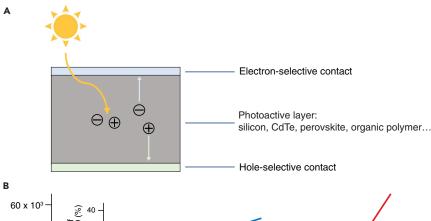
As solar materials researchers, we recognize in the history of PV development a remarkable legacy of materials innovations. When the power conversion efficiency (PCE) of back surface field silicon cells plateaued, aluminum oxide coating was developed to provide effective rear passivation. The resultant passivated emitter and rear cell (PERC) technology offers higher cell efficiencies, dominating the PV market with a share of more than 60% in 2020.² The development of passivating contacts further enabled silicon cells to reach 26.7% PCE, only approximately two to three points from this material's limits.

In thin film technologies such as cadmium telluride (CdTe), breakthroughs in materials processing, such as anion alloying and elimination of cadmium sulfide (CdS) layer, broke ten years of stagnation in efficiency.⁶ CdTe has reached 22.1% PCE, copper indium gallium selenide (CIGS) 23.4%, and organic solar cells recently 18.2%, all thanks to advances in materials design, synthesis, and fabrication. Perovskite

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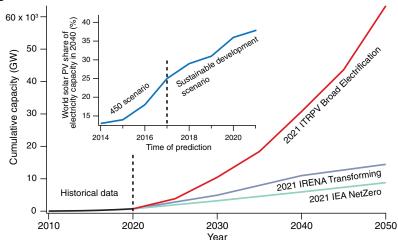


Figure 1. Challenges associated with upscaling present opportunities for materials research (A) Typical architecture of a solar cell.

(B) Models predicting multi-terawatt solar PV deployment for net zero by 2050. Inset: projected world solar PV shares by IEA World Energy Outlook since 2014. 1

solar cells have risen from below 10% PCE in 2010 to 25.7% PCE today, leaving only a one-point gap relative to the best silicon cells.

What can we, the materials research and development community, do to continue the advance of PV innovations and thus to contribute to $\leq 1.5\,^{\circ}\text{C}$ warming by mid-century? We need to continue advancing high-performance materials and architectures that demonstrate reliability and that are scalable and low cost and we need to do so within the limited time available to us. The benchmark to beat is c-Si PV, which not only has high efficiencies ($\sim 23\%$ in panels) and demonstrated reliability (~ 20 years), but is also low cost ($\sim 0.20\$/W$).

High efficiency

Improved cell PCE increases the generated power. Increased generation has the greatest impact on electricity prices because it cuts several important costs at once: land acquisition, inverters, and mounting structures. This makes high efficiency the key to terawatt-scale PV. For most solar cells, efficiency is limited by voltage loss due to non-radiative recombination at the contact interface and grain boundary. For example, all high-efficiency silicon cells require a passivating contact, and record-breaking perovskite solar cells employ ammonium ligand treatments to passivate the top surface. However, frequently used metal oxide and organic passivants, such as Al₂O₃ and trioctylphosphine oxide (TOPO), are

insulating in nature, which impedes charge transport. Further research is required to understand interfacial science and to develop novel materials to enable defect passivation without compromise.

Decades of development have brought c-Si PV performance close to its thermodynamic limit. Technologies such as perovskite and CIGS suffer the same limit. It is thus advanced architectures that move into new physical regimes, unlocking the needed step change in PCE. Multi-junction cells combine absorbers with multiple bandgaps to reduce thermalization loss. Until now, because wide-bandgap absorber options have been limited, multi-junctions have relied largely on III-V materials. In recent years, though, we have seen rapid progress in perovskite-based tandem cells. Widebandgap perovskite top cells can be customized to pair with silicon, CIGS, organics, and narrow-bandgap lead-tin (PbSn) perovskite cells. Perovskite/silicon tandems recently reached an impressive 29.8% PCE. Though triple junctions offer a long-term path to even higher theoretical efficiency (>50%), perovskite-based triple-junction cells are much less reported, the result of severe light-induced instability and interfacial non-radiation recombination in 2.0 eV bandgap perovskites. New materials strategies to mitigate halide segregation and perovskite and selective-contact interfacial loss need to be developed.

The bifacial cell offers also to increase overall solar energy harvesting. Replacing the opaque back electrode with a transparent one enables the collection of diffuse light from the rear side of the cell, adding up to 8% relative power gain atop monofacial cell figures⁷. The market share for bifacial cells is expected to grow from 30% in 2020 to near 80% by 2031.² The effect of bifaciality on energy yield in multi-junctions is an important topic for further study because two-terminal tandems require current matching between the top and



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bottom cells. Temporal variation in the intensity of diffused light due to changes in lighting condition will perturb current matching between top and bottom cells, causing a drop in tandem power output. Though the fill factor is seen to increase in the current-mismatched conditions, compensating for the current drop, further research is needed to clarify such effects, especially in perovskite-based multi-junctions.

Reliability science

Solar cell reliability is directly linked to the LCOE and the energy payback time. Without a lifetime comparable to silicon panels (~20 years), emerging technologies will be hard placed to contribute to PV at scale. For instance, most highly efficient perovskite solar cells (>24%) decay to 80% of initial PCE (T_{80}) after continuous maximum point tracking of 1,000 h. Even with an advantage in production cost, perovskite cells will need at least \sim 14-year lifetimes to reach parity with the LCOE of silicon.⁸ Research and development efforts must be targeted toward understanding the reliability science of perovskite solar cells.

Photovoltaic devices in the field operate in a multi-stressor space: oxygen, moisture, UV light, visible light, temperature cycling, and electrical bias. However, reported emerging PV degradation data typically only employ one to two stressors. Stability studies could benefit from improved description of measurement conditions and could better take advantage of common measurement standards—all of which will facilitate comparison among datasets. The incomplete understanding of emerging cell responses to mixed stressors poses a significant challenge on the path to stable device architectures. With degradation scenarios involving several mechanisms and timescales, figures of merit such T₈₀ lifetime do not capture complex non-linear behavior.

In sum, emerging PV technologies need the next generation of degradation studies, which will require planned data capture that samples the stressor space with sufficient density to pinpoint locations and mechanisms of degradation.

Beyond fundamental research into proof-of-concept lab cells that demonstrate high efficiency and stable operation, efforts are needed to cut the capital and environmental cost of large-scale manufacturing.

Low material and processing cost

Established PV technologies rely on high-temperature materials growth and vacuum deposition processes: silicon wafer growth, selenization and sulfurization for CIGS, and vapor transport for CdTe. Emerging technologies such as organic and perovskite PV offer a different, low-temperature solution-processable fabrication route that promises to reduce not only the capital expenditure for manufacturing equipment, but also the processing cost (roll-to-roll, spray coating, ink-jet printing, slot-die coating)7. However, the PCEs of these new technologies have yet to be scaled well to large areas. For example, above 25% PCE perovskites are reported in 0.1 cm² sizes, while PCEs decrease to around 22% at 1 cm², and further reduce to below 20% at sizes exceeding 50 cm². Effort is needed to improve materials quality via scalable fabrication methods. In addition, glass substrates (as high as 50% for perovskite cells) and metallization (21% for PERC silicon cells) are among the most significant cost contributors⁷: research is needed to develop high-performance cells based on lightweight, flexible polymer substrates and new metal contacts such as copper or carbon electrodes.

Sustainability

Sustainability is critical for upscaling to multi-terawatt capacity in 2050. Elements such as silver (Ag), aluminum (Al), and indium are not only used in the PV industry but also are

heavily used in other industries. PV manufacturing at the terawatt scale could place a significant demand on overall Ag production by 2030.⁵ Though abundant and recyclable, Al deserves attention because the primary Al production is a highly energy-intensive process, and secondary Al is insufficient for the totality of projected future PV production. 9 Upscaling of CIGS and CdTe could become limited by the finite supply of indium and tellurium. The scarcity and competing applications of indium present extra challenges for transparent conductive oxidebased PV technologies. Research is needed to find alternative transparent conductive electrodes. As another critical mineral, cesium (Cs) may cause supply chain challenges for perovskite solar cells as it is now widely used in high-efficiency devices. Recently single-junction perovskite cells have been moving toward pure formamidinium (FA)-based perovskites for a bandgap closer to Shockley-Queisser limit, but Cs is still used in wide-bandgap compositions for multijunctions. It is of interest to explore Csfree perovskite compositions.

Developing recycling technologies is relevant to reducing both the direct CO₂ emission and the burden of material supply. For example, more than 50% of the greenhouse emissions emitted in the production of perovskite cells is from glass and indium tin oxide (ITO).¹⁰ Fortunately, perovskite cells are soluble in polar solvents, enabling effective recycling routes to reuse 90% of ITO and glass. Greenhouse emissions can be cut by half simply by recycling the substrate and encapsulation. In parallel, enhanced stability will further improve solar cell sustainability by minimizing recycling frequency and lower energy intensity associated with still-developing recycling procedures.

Conclusion

Given that we have fewer than 30 years until 2050, it is imperative that we act fast to address these challenges. Strategic use of artificial intelligence and

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high-throughput experiment methods can potentially accelerate materials discovery and help us shorten research timeline.

Today we have multiple options for solar technologies competing to power a cleaner world. New generations of solar cells offer distinct advantages to established ones and will disrupt the market share if challenges such as large-area synthesis and stability can be addressed. We have seen unprecedented fast progress in emerging solar PV in the past few years, and the momentum will likely continue. The solar race has not yet been won; indeed, the race has just begun.

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