

# Electronic Supplementary Information (ESI) for Pathways for Solar Photovoltaics

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## Glossary of Terms

**Balance-of-system (BOS):** All components of an installed solar PV system besides PV modules. This term typically includes both hardware (e.g., inverter, transformer, wiring, and racking) and non-hardware (e.g., installation labor, customer acquisition, permitting, inspection, interconnection, sales tax, and financing) costs.

**Bandgap:** Fundamental property of semiconducting materials that determines the minimum energy (maximum wavelength) of light that can be absorbed, in units of electron-volts (eV). Direct-bandgap materials (e.g., GaAs, CdTe, and PbS) absorb light much more efficiently than indirect-bandgap materials (e.g., Si and Ge), reducing the required absorber thickness.

**Byproduction:** Production of an element as a secondary product of the mining and refinement of a major (primary) metal. Byproduction can reduce raw material prices substantially due to economies of scope, but the associated price volatility and production ceiling make byproduced elements a potential obstacle to large-scale deployment of some PV technologies.

**Capacity factor (CF):** The ratio of the actual AC energy output [kWh/y] of a PV system to the output of an ideal system with the same nameplate capacity and no DC-to-AC conversion losses, under constant peak irradiance (1000 W/m<sup>2</sup>) and at 25°C. Capacity factors are often used to compare electric power generation systems.

**Commodity materials:** Abundant materials (e.g., glass, concrete, and steel) that are used in PV modules and systems as well as a variety of non-PV applications. The cost and availability of commodity materials are typically determined by market conditions and production capacity rather than raw abundance.

**Critical materials:** Elements used in the active absorber or electrode layers of PV cells. Critical materials are often mined as byproducts and typically have few available substitutes for a given PV technology without sacrificing performance.

**Crustal abundance:** The relative concentration of a chemical element in the Earth's upper continental crust (top ~15 km), typically reported in units of parts per million (ppm) by mass.<sup>1</sup> Oxygen and silicon are the two most abundant elements in the crust.

**Energy yield:** The actual energy output of a PV module or system divided by the nameplate DC capacity, in units of kWh/kW<sub>p</sub> or hours. The energy yield of a PV module or system over a given time period corresponds to the number of hours for which it would need to operate at peak power

to produce the same amount of energy.

**Exciton:** An electron-hole pair bound together by electrostatic attraction. Excitons are neutral quasi-particles that are formed when light is absorbed in a semiconductor; they must be separated into free charges to contribute to photocurrent. Excitons in conventional inorganic semiconductors (Wannier-Mott excitons) are weakly bound and tend to dissociate shortly after formation. Excitons in many emerging thin-film PV materials such as organic small molecules and polymers (Frenkel excitons) are more strongly confined and only dissociate when they encounter a heterojunction interface (i.e., between two energetically dissimilar materials).

**Form factor:** General term that refers to the physical characteristics of a solar cell or module, including dimensions, weight, and flexibility.

**Insolation:** A measure of the solar energy received over a given area over a given time period, typically in units of kWh/m<sup>2</sup>/day. “Insolation” is a contraction of the phrase “incoming solar radiation.” When the time unit in the denominator is omitted, the period of observation must be specified (e.g., “an average daily insolation of 4.5 kWh/m<sup>2</sup>”). The term “irradiation” is sometimes used interchangeably with “insolation.”

**Intermittency:** Temporal variation in the availability of sunlight and hence PV panel output over varying time scales, from seconds to days to seasons. Intermittency can be caused by unpredictable (stochastic) cloud cover and weather or by predictable (deterministic) diurnal, seasonal, and climatic variations.

**Irradiance:** A measure of the solar energy received over a given area, typically in units of W/m<sup>2</sup>. The average irradiance over a given time period is equal to the insolation over the same period.

**Lattice mismatch:** A situation that occurs when a crystalline semiconductor is deposited directly (epitaxially) on another crystalline material with a different lattice constant (physical dimension of repeating unit cells in a crystal). When the mismatch is large, defects (dislocations) are likely to arise, increasing recombination and decreasing PV performance. Lattice matching is a key consideration for III-V MJ solar cells, which consist of many stacked epitaxial films with different lattice constants. Lattice-mismatched approaches avoid the need for lattice matching by incorporating a “metamorphic” buffer layer with graded composition to accommodate mismatch.

**Levelized cost of energy (LCOE):** Also known as levelized cost of electricity; total cost per unit of electrical energy produced by an electric power system, in units of \$/kWh or ¢/kWh. A complete calculation of levelized cost of energy includes the effect of actual system output (as measured by the performance ratio or capacity factor), upfront capital costs, fixed and variable operation and maintenance (O&M) costs (including fuel where applicable), subsidies, financing, cost of capital, degradation, and replacement.

**Manufacturing yield:** The fraction of manufactured cells or modules that operate as desired (i.e., within a desired tolerance of targeted performance parameters). All else equal, increasing manufacturing yield reduces module cost per watt.

**Material complexity:** The number of atoms in a unit cell, molecule, or other repeating unit of a material. Material complexity is related to the degree of disorder at the nanoscale. For current PV technologies, higher material complexity often translates to lower technological maturity, material intensity, processing temperatures, and processing complexity.

**Material intensity:** Amount of raw material required per unit of PV power output, in units of

$\text{mg}/W_p$  or  $t/GW_p$ . Material intensity varies directly with active layer thickness and inversely with cell efficiency, materials utilization, and manufacturing yield.

**Materials utilization ( $U$ ):** The fraction of original source material (feedstock) that ends up in a working solar cell. The remainder ( $1-U$ ) is lost during processing. Efficient recycling of process waste can increase materials utilization.

**Multijunction cell:** A solar cell consisting of more than one charge-collecting junction. When stacked in order of decreasing bandgap, multiple junctions allow light of particular wavelength ranges to be absorbed and photovoltaic energy conversion to occur in the sub-cell that incurs minimal thermal losses for that wavelength range.

**Open-circuit voltage ( $V_{OC}$ ):** The voltage measured across the terminals of a solar cell under illumination when no load is applied. The open-circuit voltage is fundamentally related to the balance between light current and recombination current, and is thus a primary measure of the quality of a solar cell. PV technologies with high open-circuit voltages (i.e., close to the material-dependent bandgap) typically exhibit low internal losses.

**Performance ratio (PR):** The ratio of the actual AC energy output [kWh/y] of a PV system to the output of an ideal system with the same nameplate capacity and no DC-to-AC conversion losses, under local insolation conditions and at 25°C. Performance ratios are often reported for individual months or years and are helpful for identifying failure of system components. The quality factor ( $Q$ ) is the same as the performance ratio.

**Processing complexity:** A qualitative measure of the difficulty of purifying raw materials and manufacturing cells and modules for a given PV technology. Technologies with high processing complexity may require substantial capital equipment investments, many discrete manufacturing steps, high material purity, high-temperature processing, and long process times. Processing complexity tends to vary inversely with material complexity.

**Recombination:** Undesirable loss of charge carriers within a solar cell. Radiative recombination results in emission of a photon and is the basis of light-emitting device (LED) operation, while non-radiative recombination results in energy loss as heat. Recombination rates are often increased by defects in bulk semiconducting material or at interfaces.

**Roll-to-roll (R2R) processing:** General term for high-throughput film deposition on flexible substrates (e.g., papers, plastics, and textiles) in the form of continuous rolls. Roll-to-roll processing may reduce thin-film PV processing costs per area substantially, although commercial demonstrations at large scale are currently limited.

**Shockley-Queisser limit:** Maximum theoretical power conversion efficiency, originally derived by Shockley and Queisser in 1961, for a solar cell consisting of a single  $pn$  junction. This limiting efficiency depends on the assumed solar spectrum (e.g., blackbody approximation, AM0 outside Earth's atmosphere, or AM1.5G at the surface). The Shockley-Queisser or detailed balance efficiency limit is 33.7% for a bandgap of 1.34 eV, under the AM1.5G spectrum without concentration at 300 K.<sup>2,3</sup> Multijunction cells can achieve efficiencies above this value.

**Solar fraction:** The fraction of global electricity demand satisfied by solar photovoltaics.

**Specific power:** The power output per unit weight of a PV cell or module, in units of W/g. Thin-film solar cells can achieve higher specific power than wafer-based cells based on active layer weight alone, but substrate weight often dominates the specific power of today's thin-film cells.

## Life Cycle Carbon Intensity of PV

The carbon footprint of solar PV (in grams of CO<sub>2</sub>-equivalent per kWh of electricity produced [g CO<sub>2</sub>-eq/kWh]) depends on both the electricity generated and the greenhouse gases (GHGs) emitted throughout the PV life cycle. A full life cycle assessment (LCA) tracks the complete environmental burden of PV—including material and energy flows—from upstream processes (i.e., materials extraction and processing, module and system component manufacturing, transportation, and installation) through 20–30 years of operation to downstream processes (i.e., plant decommissioning, recycling, and waste disposal).<sup>4-13</sup>

The life cycle carbon intensity of PV is typically dominated by emissions from the energy consumed during materials extraction and component manufacturing.<sup>4</sup> Ignoring differences in manufacturing energy consumption and installed system performance with location, we can roughly estimate the relative impact of manufacturing location and deployment location on the carbon footprint of c-Si PV. For this example, we consider the United States and China as representative locations for PV manufacturing and deployment. We acknowledge that a proper life cycle calculation for PV considers many more factors than those described in the equations below.<sup>14,15</sup> However, we adopt a simplistic approximation below, to elucidate the principal parameters that often govern life cycle calculations.

**Life cycle carbon intensity of PV ≈ “Levelized” carbon footprint of PV manufacturing**

$$C_{PV} \approx C \times E \times \left(\frac{1}{Y}\right)$$

$$\left[\frac{\text{g CO}_2\text{-eq}}{\text{kWh}}\right] = \left[\frac{\text{g CO}_2\text{-eq}}{\text{kWh}}\right] \times \left[\frac{\text{kWh}}{W_p}\right] \times \left[\frac{W_p}{\text{kWh}}\right]$$

where  $C_{PV}$  = life cycle carbon intensity of PV

$C$  = carbon intensity of local electricity<sup>16</sup>

$$C_{US} = 610 \text{ g CO}_2\text{-eq/kWh}$$

$$C_{China} = 1049 \text{ g CO}_2\text{-eq/kWh}$$

$E$  = energy required to manufacture 1  $W_p$  of PV

$Y$  = energy yield ( $1/Y = W_p$  required to get 1 kWh of lifetime output)\*

A 2012 LCA harmonization study by Hsu *et al.*<sup>4</sup> screened a broad range of published c-Si PV LCAs and adjusted their estimates of life cycle GHG emissions to correct for different values of input parameters, including insolation, module efficiency, performance ratio, and system lifetime<sup>†</sup>. The analyses referenced in that study were published between 2000 and 2009, and as a result rely primarily on data from PV manufacturers in Europe and in the U.S. For an annual insolation of 1,700 kWh/m<sup>2</sup>/y (194 W/m<sup>2</sup> or 4.7 kWh/m<sup>2</sup>/day)—corresponding to the average insolation in southern Europe—the study reports a median (harmonized) life cycle carbon

\* As mentioned above, the energy yield of a PV system depends directly on local insolation and system performance. In this analysis, we assume that the system performance is unaffected by deployment location, and hence differences in energy yield can be attributed to differences in insolation.

† Hsu and colleagues report harmonized results based on an annual insolation of 1,700 kWh/m<sup>2</sup>/y, a module efficiency of 13.2% (mc-Si) or 14.0% (sc-Si), a performance ratio of 0.75 (rooftop and building-integrated systems) or 0.80 (ground-mounted systems), and a system lifetime of 30 years.

intensity of 45 g CO<sub>2</sub>-eq/kWh, with an interquartile range of 39–49 g CO<sub>2</sub>-eq/kWh.

As shown in **Figure 2** in the main text, the average irradiance in the continental U.S. ranges from 135–245 W/m<sup>2</sup> (3.2–5.9 kWh/m<sup>2</sup>/day). Correcting for differences in insolation gives an estimated range for the median carbon intensity of c-Si PV modules manufactured in the U.S. and deployed in the U.S.: **36–65 g CO<sub>2</sub>-eq/kWh**. If the primary factor contributing to life cycle GHG emissions is the carbon intensity of electricity in the manufacturing location, we can scale the values above by the ratio of the average carbon intensities of electricity in China and in the U.S. ( $\frac{C_{China}}{C_{US}} = \frac{1049}{610}$ ) to estimate the carbon intensity of PV modules manufactured in China and deployed in the U.S.: **61–111 g CO<sub>2</sub>-eq/kWh**.

The average irradiance in China ranges from 125–265 W/m<sup>2</sup> (3.0–6.4 kWh/m<sup>2</sup>/day). Performing the same adjustments as before, we calculate the carbon intensity of PV manufactured in either the U.S. or China, and deployed in China. The results are listed below.

*Carbon intensity of PV modules manufactured in U.S. and deployed in U.S.*

$$C_{PV,US,US} \approx C_{US} \times E \times \left(\frac{1}{Y_{US}}\right) \approx \mathbf{36\text{--}65 \text{ g CO}_2\text{-eq/kWh}}$$

*Carbon intensity of PV modules manufactured in **China** and deployed in U.S.*

$$C_{PV,China,US} \approx C_{China} \times E \times \left(\frac{1}{Y_{US}}\right) \approx \mathbf{61\text{--}111 \text{ g CO}_2\text{-eq/kWh}}$$

*Carbon intensity of PV modules manufactured in U.S. and deployed in **China***

$$C_{PV,US,China} \approx C_{US} \times E \times \left(\frac{1}{Y_{China}}\right) \approx \mathbf{33\text{--}70 \text{ g CO}_2\text{-eq/kWh}}$$

*Carbon intensity of PV modules manufactured in **China** and deployed in **China***

$$C_{PV,China,China} \approx C_{China} \times E \times \left(\frac{1}{Y_{China}}\right) \approx \mathbf{57\text{--}120 \text{ g CO}_2\text{-eq/kWh}}$$

All of these ranges are much lower than the typical carbon intensities of natural gas (~500 g CO<sub>2</sub>-eq/kWh) and coal (~1000 g CO<sub>2</sub>-eq/kWh).<sup>17</sup> So PV electricity is cleaner than fossil fuel-based electricity from an emissions perspective, regardless of where the modules are manufactured and deployed. But the deployment location still matters: Deploying PV in China avoids more emissions than deploying PV in the United States, due to the high carbon intensity of electricity in China today.

*Avoided emissions with PV manufactured in U.S. and deployed in **China***

$$C_{China} - C_{PV,US,China} = 1049 - (33 \text{ to } 70) = \mathbf{979\text{--}1016 \text{ g CO}_2\text{-eq/kWh (best case)}}$$

*Avoided emissions with PV manufactured in **China** and deployed in **China***

$$C_{China} - C_{PV,China,China} = 1049 - (57 \text{ to } 120) = \mathbf{929\text{--}992 \text{ g CO}_2\text{-eq/kWh}}$$

*Avoided emissions with PV manufactured in U.S. and deployed in U.S.*

$$C_{US} - C_{PV,US,US} = 610 - (36 \text{ to } 65) = \mathbf{545\text{--}574 \text{ g CO}_2\text{-eq/kWh}}$$

*Avoided emissions with PV manufactured in **China** and deployed in **U.S.***

$$C_{\text{US}} - C_{\text{PV,China,US}} = 610 - (61 \text{ to } 111) = \mathbf{499\text{--}549 \text{ g CO}_2\text{-eq/kWh}} \text{ (worst case)}$$

Thus if our goal is to reduce emissions, it is far less important **where the PV is made** (reduction of -13–87 g CO<sub>2</sub>-eq/kWh if manufactured in U.S. instead of China) than **where it is used** (380–493 g CO<sub>2</sub>-eq/kWh if deployed in China instead of U.S.), and most important **whether it is used at all** (499–1016 g CO<sub>2</sub>-eq/kWh if deployed).

# Basics of Solar Photovoltaic Energy Conversion

## Introduction

In this primer, we describe the principles governing the conversion of light into electricity in photovoltaic (PV) devices. We begin by discussing the fundamentals of energy conversion, light, and electric power. We next introduce the concept of semiconductors, describing the electrical and optical properties that govern their interaction with light. We explain the concept of the diode as the fundamental functional unit of a PV device and describe the characterization and standard performance metrics of solar cells. Finally, we discuss how solar cells are used in PV modules, arrays, and systems. For a more complete explanation of the physical concepts described here, we point the interested reader toward a number of relevant textbooks.<sup>18-24</sup>

## Energy and Power

*Energy* can be defined as the capacity of a system to perform work.\* In the International System of units, energy is measured in units of *joules* (J); 1 J is roughly the amount of energy required to lift a can of soda 1 foot off the ground.† *Power* is the rate of flow of energy per unit time and is measured in units of *watts* (W), where 1 W is equal to an energy flow of 1 J/s. Energy can thus equivalently be expressed in units of *watt-hours* (Wh) or, more commonly in the electric power sector, *kilowatt-*, *megawatt-*, *gigawatt-*, or *terawatt-hours* (kWh, MWh, GWh, and TWh, respectively). A typical home in the United States utilizes electric power at an average rate of roughly 1.24 kW, corresponding to an energy usage of ~30 kWh per day.<sup>25</sup>

Energy cannot be created or destroyed, but it can be stored and converted between different forms.‡ There are many different forms of energy: The chemical energy stored in carbon-carbon bonds in a piece of coal, the gravitational potential energy of elevated water in a dammed reservoir, and the radiant energy continually delivered to the Earth's surface by the Sun are all familiar examples. What are typically thought of as energy *generation* devices—coal-fired power plants, hydroelectric dams, or solar panels—are thus actually energy *conversion* devices.

**Fig. S1** summarizes, in a simplified format, the forms of energy and processes of energy conversion relevant to electric power generation. Note that the only continuous input of energy to the Earth is the radiant energy of the Sun. Each energy conversion process, here denoted by labeled arrows, involves the irreversible conversion of some portion of the energy input to low-grade thermal energy (i.e., waste heat). Some of these conversion processes are more efficient than others; while turbines can convert only around 30–40% of the thermal energy from burning coal into kinetic energy, generators can convert over 90% of the kinetic energy of a spinning turbine into electrical energy. Photovoltaics are unique in their ability to directly convert radiant solar energy to electrical energy, and by eliminating the relatively inefficient processes of

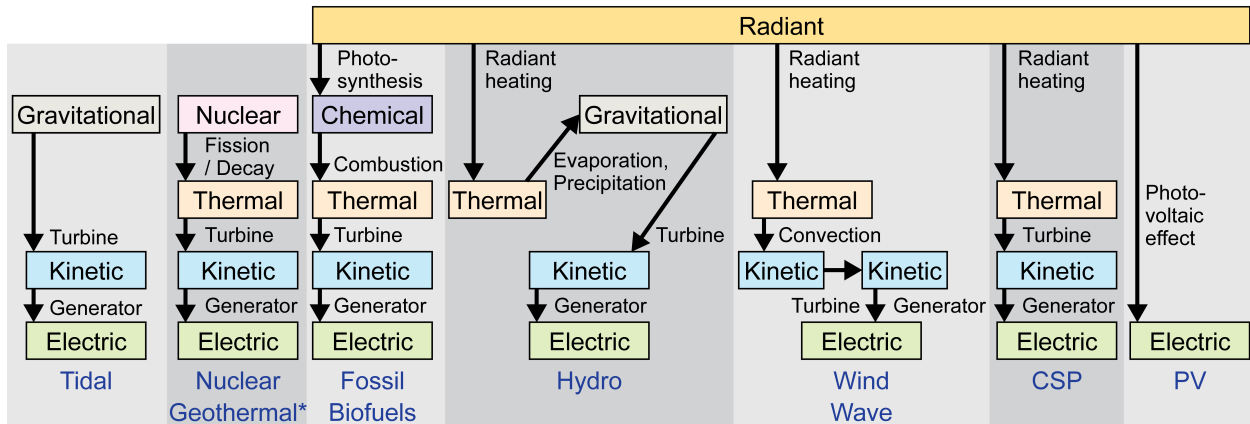
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\* We refer to *work* as it is used in physics; that is, as a measure of the force applied on a point in motion over a displacement in position, for the component of the force in the direction of that motion.

† Much more energy is contained *within* the can of soda; one joule is roughly the amount of extractable dietary energy contained in one-hundredth of a drop of soda.

‡ Einstein's famous " $E=mc^2$ " equation implies that mass and energy are equivalent properties and represent the same physical quantity—not that energy can be "created" from matter.

photosynthesis (0.5–2% efficient)<sup>26</sup> and thermal-to-kinetic-energy conversion, they represent the most direct and efficient use of Earth’s primary energy input—sunlight.



**Fig. S1:** Relevant forms of energy (colored boxes) and energy conversion processes (labeled arrows) for the production of electric power. Note that gravitational, nuclear, and chemical energy all represent energy that can be stored for long periods of time with high efficiency; direct storage of thermal, kinetic, or electric energy is much less efficient. Radiant energy from the Sun is the only external energy input to the Earth system.\*

We next describe the properties of light (radiant power) and electricity (electric power)—the input and output of PV devices, respectively.

## Light

Light refers to a specific type of *electromagnetic radiation* (EM) that is visible to the human eye. Electromagnetic radiation is comprised of alternating electric and magnetic fields that oscillate with a given *frequency* and *wavelength* and propagate in a straight line. **Fig. S2** graphically represents the EM spectrum. Visible light is typically characterized as EM radiation with a wavelength between 400 and 750 nanometers (nm);<sup>†</sup> as shown in the figure, we perceive light of different wavelengths as different colors. This range represents a small fraction of a spectrum that stretches over many orders of magnitude in wavelength (and frequency), from gamma and X rays, through ultraviolet, visible, and infrared radiation, to microwaves and radio waves.

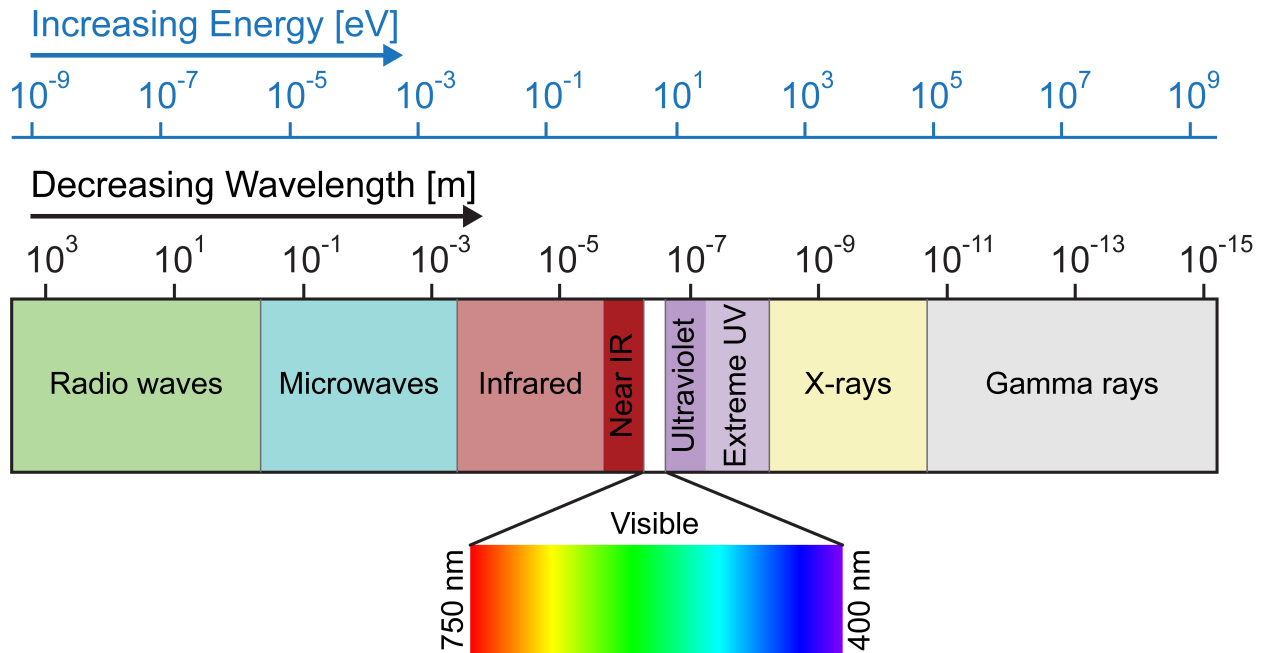
The fundamental quantized unit (or quantum) of light is the *photon*, which represents the smallest isolable packet of EM radiation of a given wavelength. The energy content of a photon is proportional to its frequency and inversely proportional to its wavelength, and the power delivered by a light source to an absorbing surface is equal to the flux, or rate of flow, of photons absorbed by that surface times the energy of each incident photon. Most of the sun’s emission spectrum lies between the ultraviolet and the infrared. The power delivered by solar radiation to a surface pointing toward the Sun, located at the Earth’s surface at noon, on a cloudless day and at a latitude representative of many of the world’s major population centers, is roughly 1000

\* The flow of geothermal energy from the Earth’s interior to its surface results in roughly equal measure from leftover energy still being dissipated from the Earth’s formation and from the nuclear decay of radioactive isotopes in the Earth’s interior.<sup>27</sup>

† One nanometer is  $10^{-9}$  m; a human hair is roughly 75,000 nm in diameter.<sup>28</sup>



$\text{W/m}^2$ , typically known as 1 sun. The nature of sunlight and its interaction with the Earth and its atmosphere is described in detail in Ref. 29.



**Fig. S2:** Spectrum of electromagnetic radiation in units of energy (in electron-volts,  $eV$ , where  $1 eV \approx 1.6 \times 10^{-19} J$ ) and wavelength (in  $\text{nm}$ ), with the visible range of light highlighted. Reprinted with permission from Ref. 30.

### Equation 1: Photon Energy

The energy of a photon  $E$  is given by

$$E = \frac{hc}{\lambda} = h\nu$$

where  $h$  is Planck's constant ( $\sim 6.63 \times 10^{-34} \text{ J}\cdot\text{s}$ ),  $c$  is the speed of light in vacuum ( $299,792,458 \text{ m/s}$ ),  $\lambda$  is the photon wavelength, and  $\nu$  is the photon frequency.

## Electricity and Electric Power

Electricity is characterized by *voltage* and *current*. Current, measured in *amperes* or *amps* (A), corresponds to the rate of flow of charge; if we imagine electricity flowing through a wire in analogy to water flowing through a pipe, current is the rate of flow of the water. Voltage, measured in *volts* (V), corresponds to the electric potential energy difference, per unit charge, between two points. In our analogy of water flow, the voltage between two points corresponds to the pressure or height difference between those points; it is the driving force behind the flow. The electrical *resistance* of a sample of material, measured in *ohms* ( $\Omega$ ), is the ratio between the voltage applied to the sample and the current that flows through it; in our analogy, the resistance would be inversely proportional to the diameter of the pipe through which the water flows. Electric power is equal to the product of voltage and current.

### Equation 2: Ohm's Law

Current  $I$ , voltage  $V$ , and electrical resistance  $R$  are related by Ohm's Law:

$$V = IR$$

We now describe the properties of charge carriers within electronic materials and explain how these materials can be used to fabricate solar cells.

### Electronic Materials

A typical solid such as silicon contains roughly  $7 \times 10^{23}$  electrons/cm<sup>3</sup> of material, where an *electron* is a subatomic particle with an electric charge, by definition, of  $-1 e$ .<sup>\*,†</sup> These electrons occupy states of well-defined energy within the solid; much like water filling up a bucket, electrons minimize their energy by filling up the lowest-energy states (the deepest part of the bucket, or the most tightly-bound atomic energy states) first.

Electrons are one of two types of charge carriers in a solid; the other is the *hole*, which is simply the absence of an electron in a position where an electron would normally be found. If electrons are compared to drops of water, holes can be compared to bubbles below the water's surface. Since it carries an absence of negative charge while surrounded by a sea of negatively charged electrons,<sup>‡</sup> a hole can be treated as a carrier of positive charge, moving in the opposite direction from an electron under an applied electric field. The *electrical conductivity* of a material is proportional to the volume density [cm<sup>-3</sup>] of mobile electrons and holes multiplied by their *drift mobility* [cm<sup>2</sup>/(V-s)] in that material, defined as the ratio of a charge carrier's velocity to the magnitude of the electric field that drives its motion.

### Equation 3: Electrical Conductivity

The electrical conductivity  $\sigma$  of a material is given by

$$\sigma = \sigma_e + \sigma_h = q(n\mu_e + p\mu_h)$$

where  $\sigma_e$  and  $\sigma_h$  are the electron and hole conductivities, respectively;  $q$  is the charge of the electron;  $n$  and  $p$  are respectively the electron and hole densities; and  $\mu_e$  and  $\mu_h$  are respectively the electron and hole mobilities.

Electrons can be *excited* by the absorption of external energy in the form of light or heat. A single excitation generates both an electron and a hole; the excited electron transfers to a higher-energy state and leaves a hole in its previous state. In a typical solid at room temperature, heat is manifested as minute vibrations in the atoms that make up the solid. For electrons, this heat behaves like a continuous spectrum of low-energy excitations, inducing small ripples on the surface of the energetic sea of electrons.

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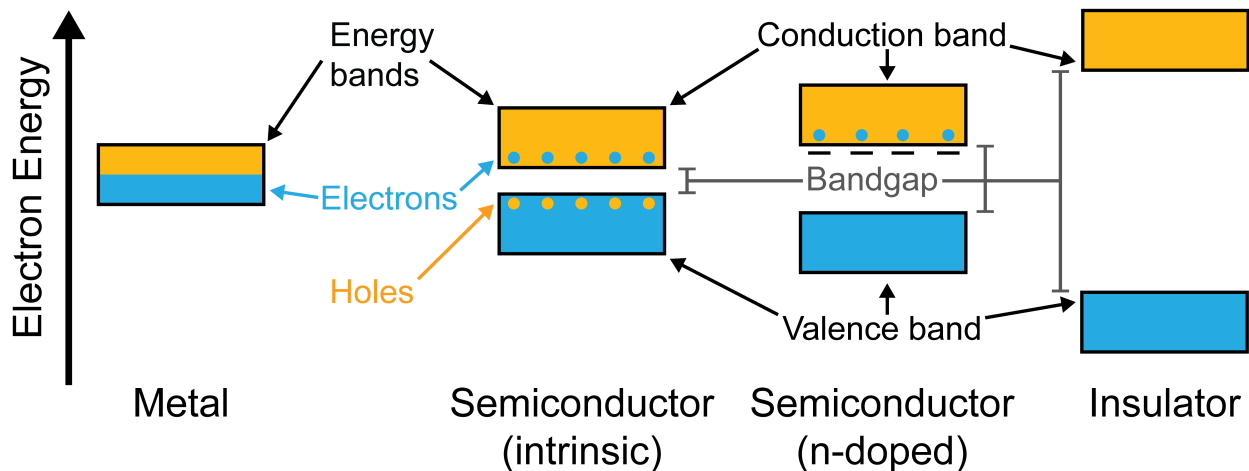
\* A charge of "1 e" is equivalent to  $\sim 1.6 \times 10^{-19}$  A-s, or the amount of charge that flows past a point when a current of 1 A is allowed to flow for  $\sim 1.6 \times 10^{-19}$  s.

† An electron-volt (eV) can also be defined as the energy gained by an electron as it passes through a voltage difference of 1 V.

‡ The negative charge of each electron is balanced by a positive charge in the nucleus of the atom from which the electron originates, such that the entire solid carries no net charge.

Like vibrational modes on a guitar string, only certain electron energies are allowed within a material. In a single atom or molecule, these energies exist as discrete, isolated energy states; in extended many-atom solids, these discrete states are smeared out into broad *energy bands*. In pure materials, electrons can only reside at energies within these bands; they cannot occupy energies between bands, where there are no electronic states. The electronic properties of a material are determined to a large extent by the shapes of these bands and the extent to which they are filled with electrons. The highest-energy band that is completely filled with electrons is called the *valence band*; the next-higher band is called the *conduction band*.

As shown in **Fig. S3**, the three major classes of electronic materials—*metals*, *insulators*, and *semiconductors*—are characterized by distinct energy band arrangements. *Metals* contain an incompletely filled energy band, allowing electrons at the energetic surface of the filled states to move (much like waves in a partially-filled container of water). *Insulators* contain completely filled bands separated by a large energy *bandgap*. This bandgap in insulators is too wide to allow significant excitation of electrons across the gap by heat (at typical operating temperatures) or visible photons. Because the valence band of insulators is completely filled with electrons (with no mobile holes) and the conduction band is completely empty of electrons, no charge carriers are available to flow under an applied electric field, making these materials electrically resistive. *Semiconductors* are intermediate between metals and insulators; they exhibit a bandgap that is small enough for electrons to be excited across it by heat or visible photons. Most importantly, semiconductors can be *doped* (intentionally or unintentionally) with minute quantities of foreign atoms that donate excess electrons or holes to the rest of the solid. Doping allows the density of free charge carriers and thus the conductivity of the material to be controlled over many orders of magnitude.



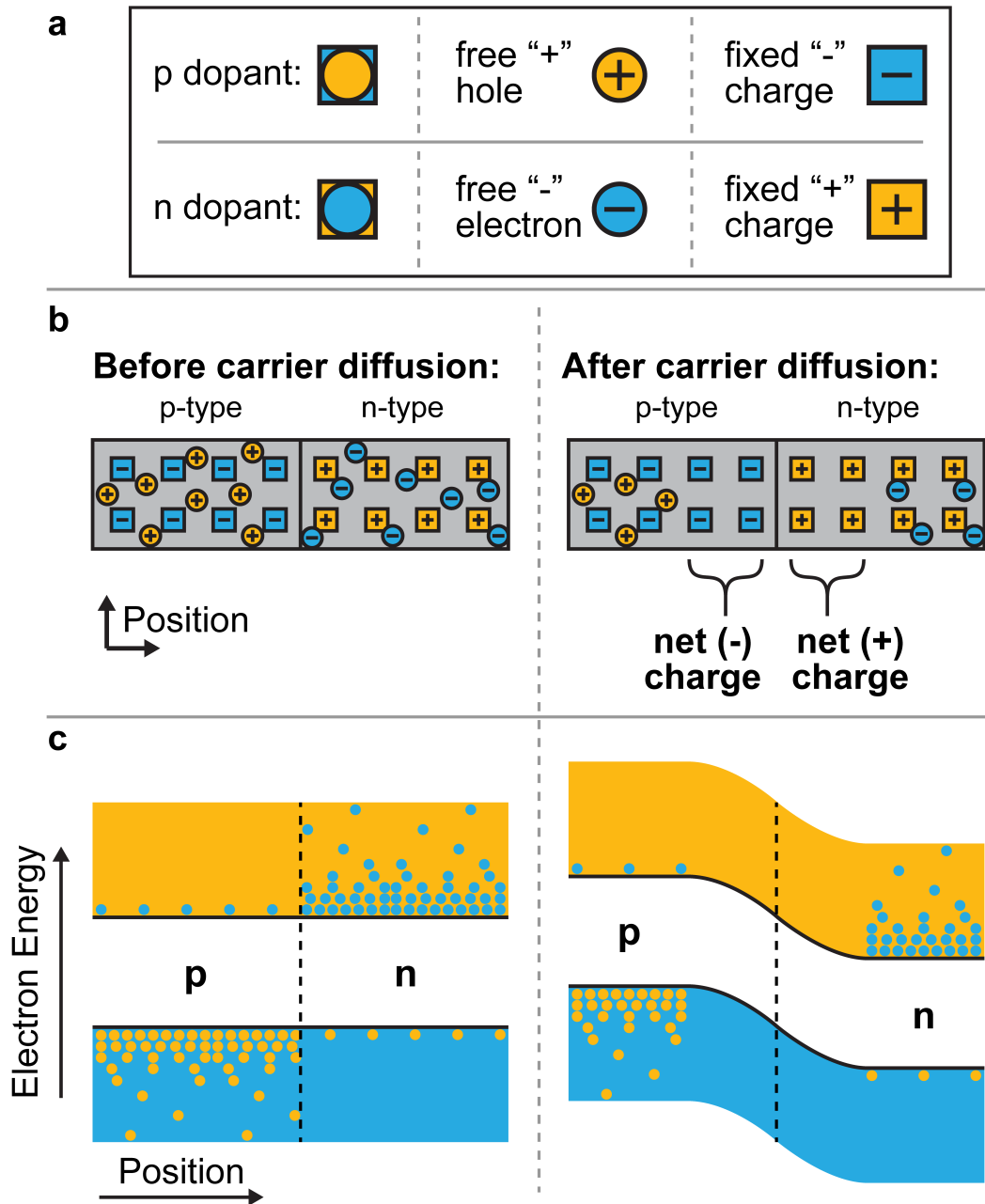
**Fig. S3:** Schematic electronic band structure of metals, semiconductors, and insulators.

**Table 1:** Bandgaps of various materials. Common solar cell materials are highlighted in blue; insulators are highlighted in green.<sup>20,22,31-33</sup>

Material	Bandgap [eV]
Metals	0
PbS (lead sulfide)	0.4
Si (silicon)	1.1
CdTe (cadmium telluride)	1.4
CIGS (copper indium gallium diselenide)	1.0–1.7
C (diamond)	5.5
SiO <sub>2</sub> (silica glass)	~9
LiF (lithium fluoride)	13.6

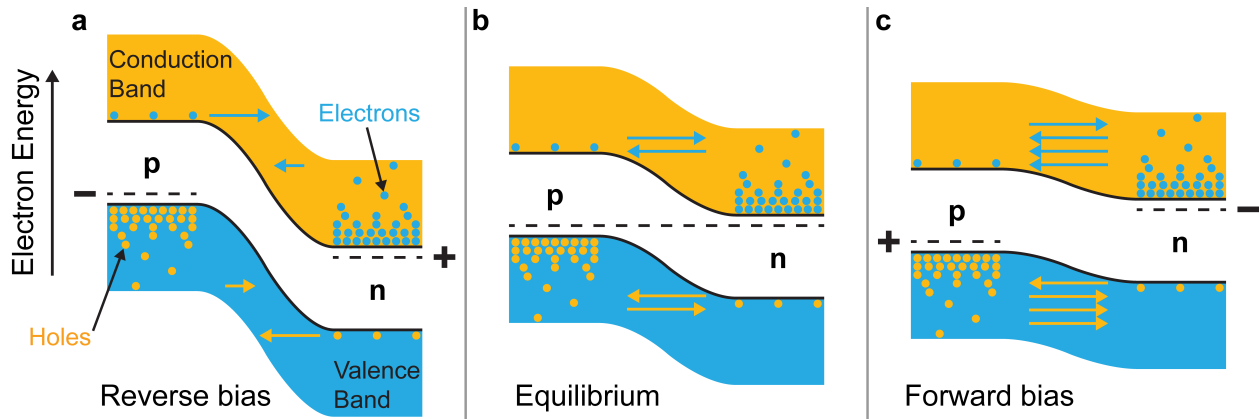
### ***pn*-Junction Diodes and Solar Cells**

The fundamental functional unit of a solar cell is a *pn-junction diode*, which forms at the interface between two semiconductors: one doped with an excess of electron-donating impurities (an *n-type* semiconductor, so named for the excess of free *negatively*-charged electrons), and one doped with an excess of hole-donating impurities (a *p-type* semiconductor, so named for the excess of free *positively*-charged holes). **Fig. S4** illustrates the fundamentals of the *pn*-junction diode. When an *n*-type and *p*-type material are put in contact, free electrons from the *n*-type side and free holes from the *p*-type side diffuse across the interface, cancelling each other out (the electrons “fill in” the holes). This elimination of the free carriers near the interface uncovers the fixed charges of the dopants that originally balanced the charge of the free electrons and holes, generating a built-in electric field in the interface region that prevents further diffusion. This field corresponds to a built-in voltage between the *n*-type and *p*-type sides of the junction.

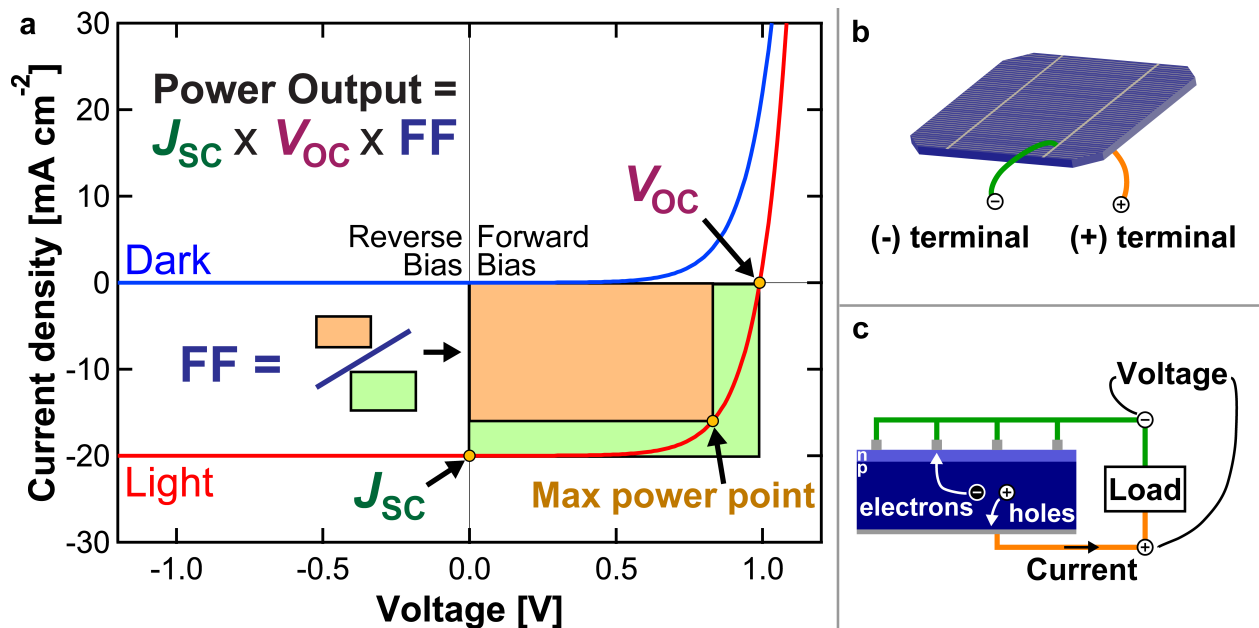


**Fig. S4:** Physical structure and electric properties of a *pn*-junction diode before and after diffusion of charge carriers across the junction interface.

The diode acts as a one-way valve for charge carriers, as shown in **Fig. S5**. If a positive voltage is applied to the *p*-type side of the junction (forward bias), the built-in field is reduced, and large numbers of carriers can diffuse across the interface, generating a large current. If a negative voltage is applied to the *p*-type side (reverse bias), the built-in field is strengthened, diffusion remains unfavorable, and the current remains low. The current flow in a representative diode at different applied voltage levels is shown by the curve labeled “dark” in **Fig. S6a**: The current increases exponentially under positive voltage, but remains small under negative voltage.



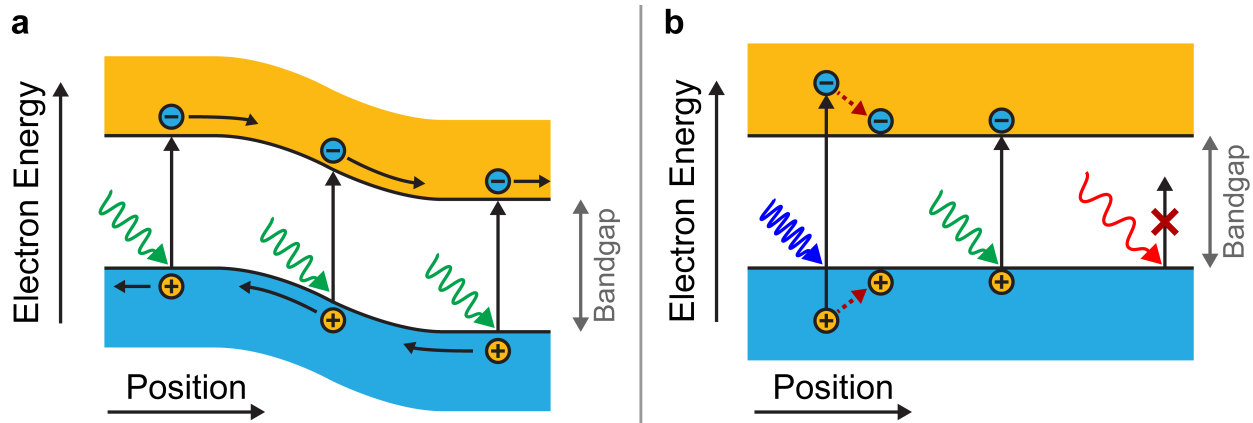
**Fig. S5:** Energy band diagram during operation of a pn-junction diode in the dark, showing (a) reverse bias, (b) equilibrium, and (c) forward bias conditions. Blue and orange arrows represent flux of electrons and holes, respectively.



**Fig. S6:** (a) Representative current-voltage characteristics of a solar cell in the dark (blue curve) and under illumination (red curve). The short-circuit current density ( $J_{SC}$ ), open-circuit voltage ( $V_{OC}$ ), and fill factor ( $FF$ ) are indicated; the physical significance of these metrics is described in the text. Since the current output of an illuminated solar cell is proportional to its illuminated surface area, the current density (current divided by area) normalizes for different cell sizes. Voltage and current are measured between the positive and negative terminals of the solar cell (b, c).

A solar cell is simply a diode that can generate free electrons and holes through the absorption of light, as depicted in **Fig. S7a**. These free charge carriers are separated under the built-in electric field of the diode, generating photocurrent. Since the generation of photocurrent is roughly independent of the voltage across the solar cell, the “light” curve in **Fig. S6** is vertically offset by

a constant amount from the “dark” curve. The current is correlated with the number of carriers generated, which depends upon the absorption properties of the semiconductor and its efficiency in turning absorbed photons into extractable charge carriers (this efficiency, known as the *external quantum efficiency (EQE)*, is described in more detail below). The voltage is correlated with the strength of the built-in electric field of the diode.



**Fig. S7:** (a) Operation of a solar cell under illumination, showing excitation of electrons and holes by light, followed by charge carrier separation under the built-in electric field. The conduction band and holes are shown in orange; the valence band and electrons are shown in blue. (b) Interaction of light of various wavelengths with a light-absorbing semiconductor. Short-wavelength photons of energy higher than the bandgap (here depicted as blue wavy arrows) generate excited electron-hole pairs with net energy greater than the bandgap, but the electron and hole quickly lose their excess energy and “relax” to the bottom of the conduction band (for electrons) and top of the valence band (for holes). Long-wavelength photons of energy lower than the bandgap (here depicted as red wavy arrows) are not absorbed and do not generate free electron-hole pairs.

**Fig. S6** illustrates the current-voltage output of a representative solar cell both in the dark (blue curve, acting as a simple diode) and under illumination (red curve), with key operational parameters identified. If the two terminals of an illuminated solar cell are left open (i.e., not connected to each other by a conductive path) and no current is allowed to flow, the voltage measured between them is the *open-circuit voltage* ( $V_{OC}$ ). If the two terminals are shorted together by a highly conductive pathway (like a copper wire) and thus held at the same voltage, the current flowing through that pathway—divided by the cell area—is the *short-circuit current density* ( $J_{SC}$ ).

#### Equation 4: Current-Voltage Characteristics of a Solar Cell

The current density output from a solar cell,  $J_{PV}$ , as a function of voltage is given by

$$J_{PV} = J_0 \left( e^{\frac{qV}{k_B T}} - 1 \right) - J_{SC}$$

where  $J_0$  is the reverse saturation current density [ $\text{mA}/\text{cm}^2$ ],  $q$  is the charge of the electron,  $V$  is the applied voltage,  $k_B$  is the Boltzmann constant ( $1.38 \times 10^{-23}$  J/K),  $T$  is the temperature [K], and  $J_{SC}$  is the short-circuit current density [ $\text{mA}/\text{cm}^2$ ]. With  $J_{SC}$  set to zero, this equation represents the output of a simple diode.

The voltage across the terminals of an operating solar cell can range between zero and  $V_{OC}$ ; the current output stays roughly constant over much of this range, until the voltage approaches  $V_{OC}$ . The power output at a given voltage is equal to the product of the current and the voltage and will reach a maximum near the apparent “shoulder” in the current-voltage curve (as depicted by the orange rectangle in **Fig. S6**). The ratio between the power output per area at this *maximum power point* and the product of the  $J_{SC}$  and  $V_{OC}$  is the *fill factor*, which corresponds to the “squareness” of the illuminated current-voltage curve. The *power conversion efficiency (PCE)* is equal to the product of the short-circuit current density, open-circuit voltage, and fill factor, divided by the power per area of the incident light source (usually measured under standard illumination conditions of  $1000 \text{ W}/\text{m}^2$ , as discussed above).

#### Solar Cell Efficiency

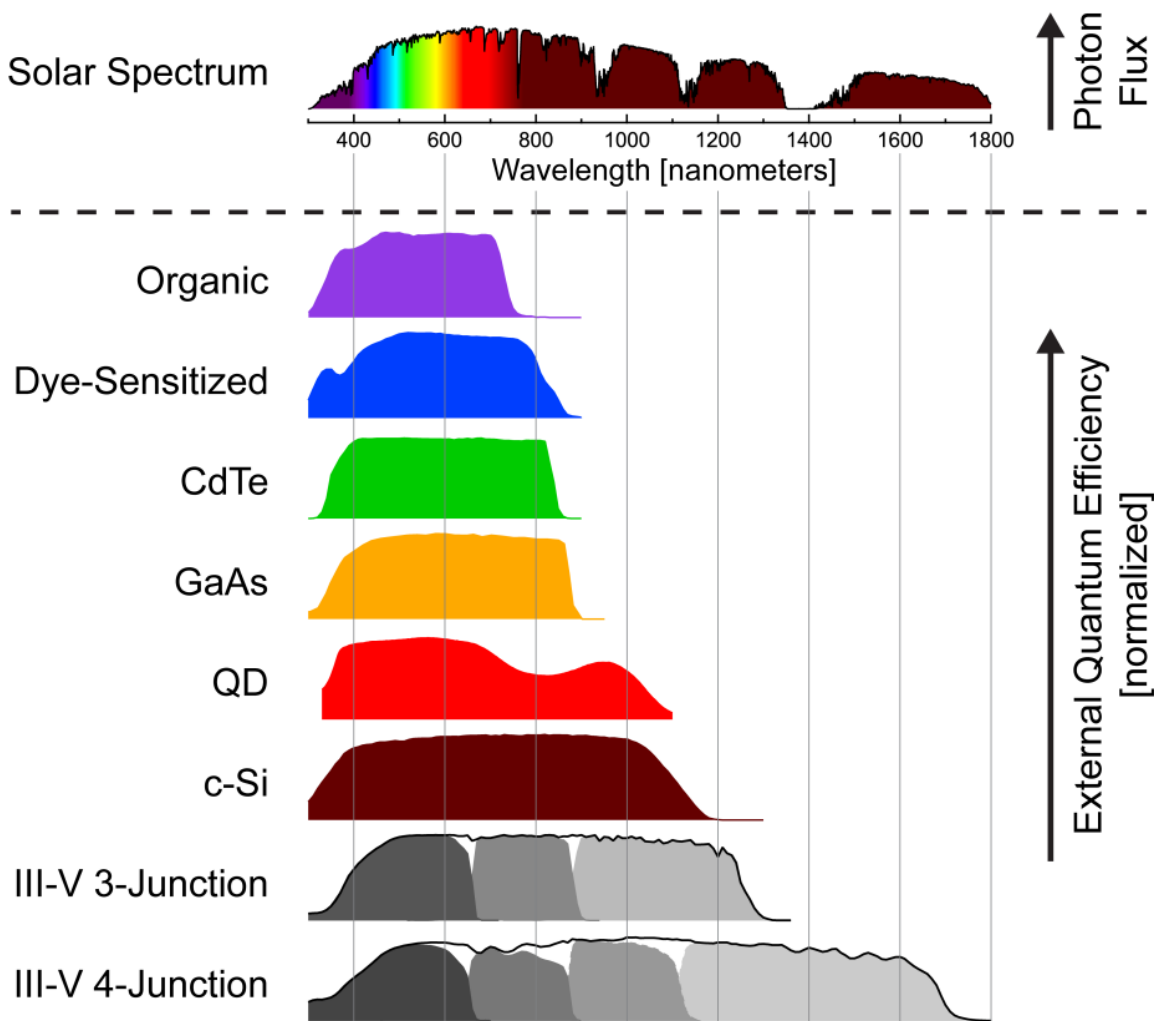
The current and voltage output of a solar cell cannot be simultaneously optimized. Since a solar cell can only absorb photons with energy greater than the bandgap, reducing the bandgap generally increases current. However, as depicted in **Fig. S7b**, electrons excited by photons with energy greater than the bandgap quickly dissipate their excess energy as wasted heat, ultimately settling at an energy equal to the bandgap. The bandgap energy is thus the maximum energy that can be extracted as electrical energy from each photon absorbed by the solar cell. Reducing the bandgap leads to smaller voltages, eventually counteracting the benefit of increased current. The broad emission spectrum of the sun thus limits our ability to harvest both the maximum number of photons and the maximum energy from each photon.

The maximum power conversion efficiency of a *single-junction* solar cell, under unconcentrated solar illumination and room-temperature operation, is roughly 33%, a quantity known as the *Shockley-Queisser Limit*.<sup>2,3</sup> This limit can be surpassed by *multijunction* solar cells that use a combination of materials of different bandgaps; these devices enable a greater fraction of the energy of each absorbed photon to be extracted as voltage and have demonstrated efficiencies up to 46% under concentrated sunlight. In an actual solar cell, the presence of defects and parasitic resistive losses decreases the efficiency to values below the theoretical limits.

As mentioned above, the external quantum efficiency of a solar cell is the efficiency with which individual photons of a given wavelength are converted to extractable charge carriers. **Fig. S8** shows the EQE spectra of world-record solar cells of various types, compared with the solar spectrum observed at the Earth’s surface. A sharp cutoff in EQE is observed on the high-wavelength (low-energy) side of each spectrum at the bandgap of the absorbing material, as photons with energy less than the bandgap cannot be absorbed. The multiplicative product of the



EQE spectrum and the solar spectrum, integrated over all wavelengths, is proportional to the short-circuit current produced by the solar cell. Incomplete absorption of the incident light by the solar cell active material may result from light reflection and from absorption by non-current-generating materials within the cell. These absorption losses, along with parasitic resistances, decrease the EQE to below 100%.



**Fig. S8:** Solar photon flux at the Earth's surface as a function of wavelength, and normalized external quantum efficiency spectra for different solar cells.<sup>34-38</sup> The solar cell technologies listed here are described in more detail in the main text.

## Solar Cell Fabrication

A solar cell can be fabricated by one of two general methods: modification of a bulk wafer or additive deposition of thin films onto a substrate. The first approach, wafer modification, is used for conventional crystalline silicon cells and III-V multijunction cells. In this method, an extremely pure wafer of semiconductor is used as the starting material and dopants are introduced near the surface to create a *pn* junction. The wafer serves as both light absorber and substrate; charge carriers are generated within the wafer and extracted directly from the front

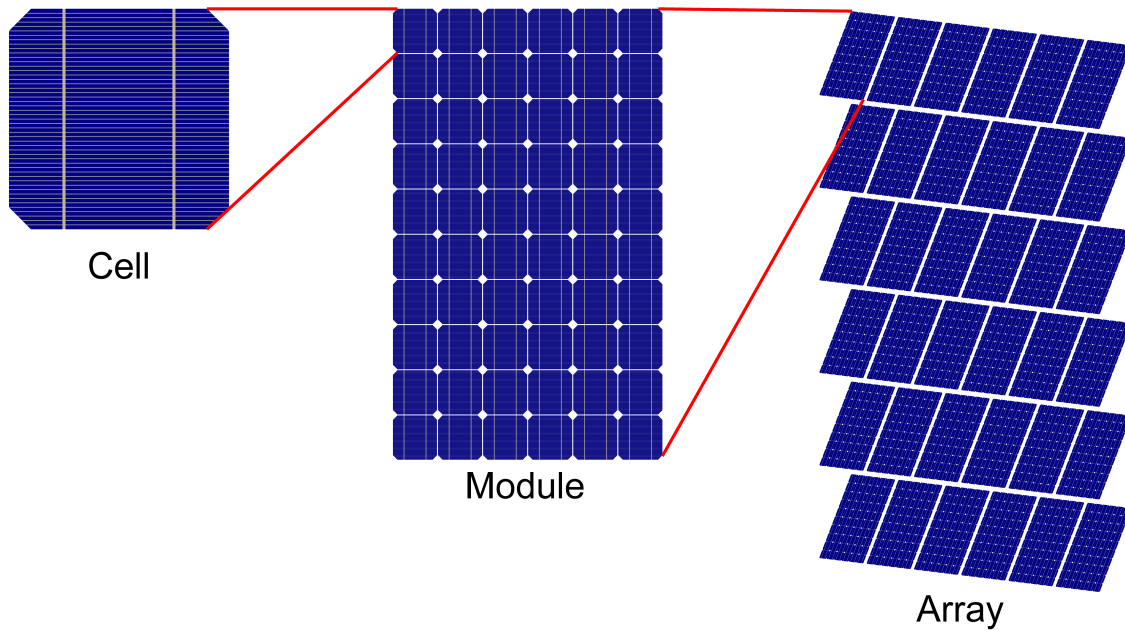
(top) and back (bottom) faces of the wafer by electrical contacts. The second approach, additive deposition, is used to make most thin-film solar cells. Here a separate substrate—a sheet of glass, plastic, or metal, which can be either rigid or flexible—serves as a mechanical support for the active cell. Light-absorbing films and electrical contacts are formed in a layer-by-layer process on the substrate by vapor- or solution-based deposition techniques such as thermal evaporation, chemical vapor deposition, spray coating, or screen printing. Different materials can be individually optimized for light absorption and charge transport, and additional layers are often introduced to enhance charge extraction.

## Solar PV Arrays and Systems

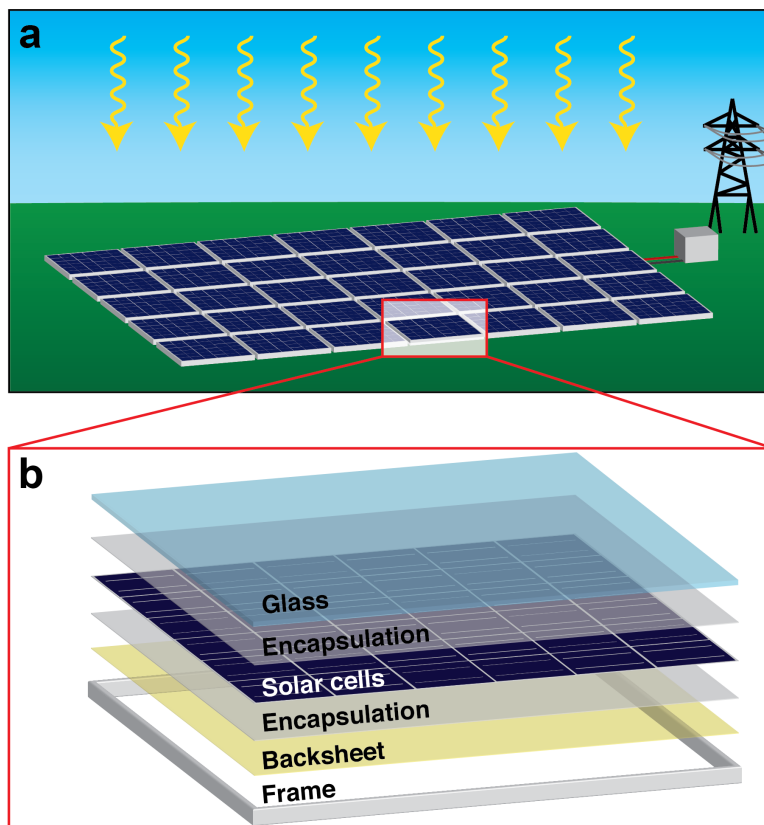
A single 6" × 6" (15 cm × 15 cm) crystalline silicon solar cell generates a voltage of ~0.5–0.6 V and a power output of ~4–5 W under illumination with direct sunlight at an intensity of 1000 W/m<sup>2</sup>. As shown in **Fig. S9**, individual cells are connected in *series* in a PV *module* or *panel* to increase their collective voltage output; a typical module contains 60 to 72 individual cells, generating a voltage of 30–48 V and a power output of 260–320 W. PV modules often incorporate additional materials, such as a glass sheet for mechanical support and protection, laminated encapsulation layers (commonly ethylene vinyl acetate, or EVA) for UV and moisture protection, a fluoropolymer backsheets for further environmental protection, and an aluminum frame for mounting (**Fig. S10**). Common module dimensions are 1 m × 1.5 m × 4 cm.

PV modules are typically connected in series to further increase their collective output voltage, or in *parallel* to increase their collective output current; such a collection of PV modules is often called a solar PV *array*. PV arrays can be stationary or can utilize solar tracking, whereby the modules are rotated throughout the day to point toward the sun, increasing the power output per panel. Some arrays—particularly those utilizing multijunction solar cells—use mirrors or lenses to concentrate sunlight onto the solar cells. Concentrating systems allow smaller solar cells to be used, but typically require accurate solar tracking to keep the concentrated sunlight focused onto the cells.

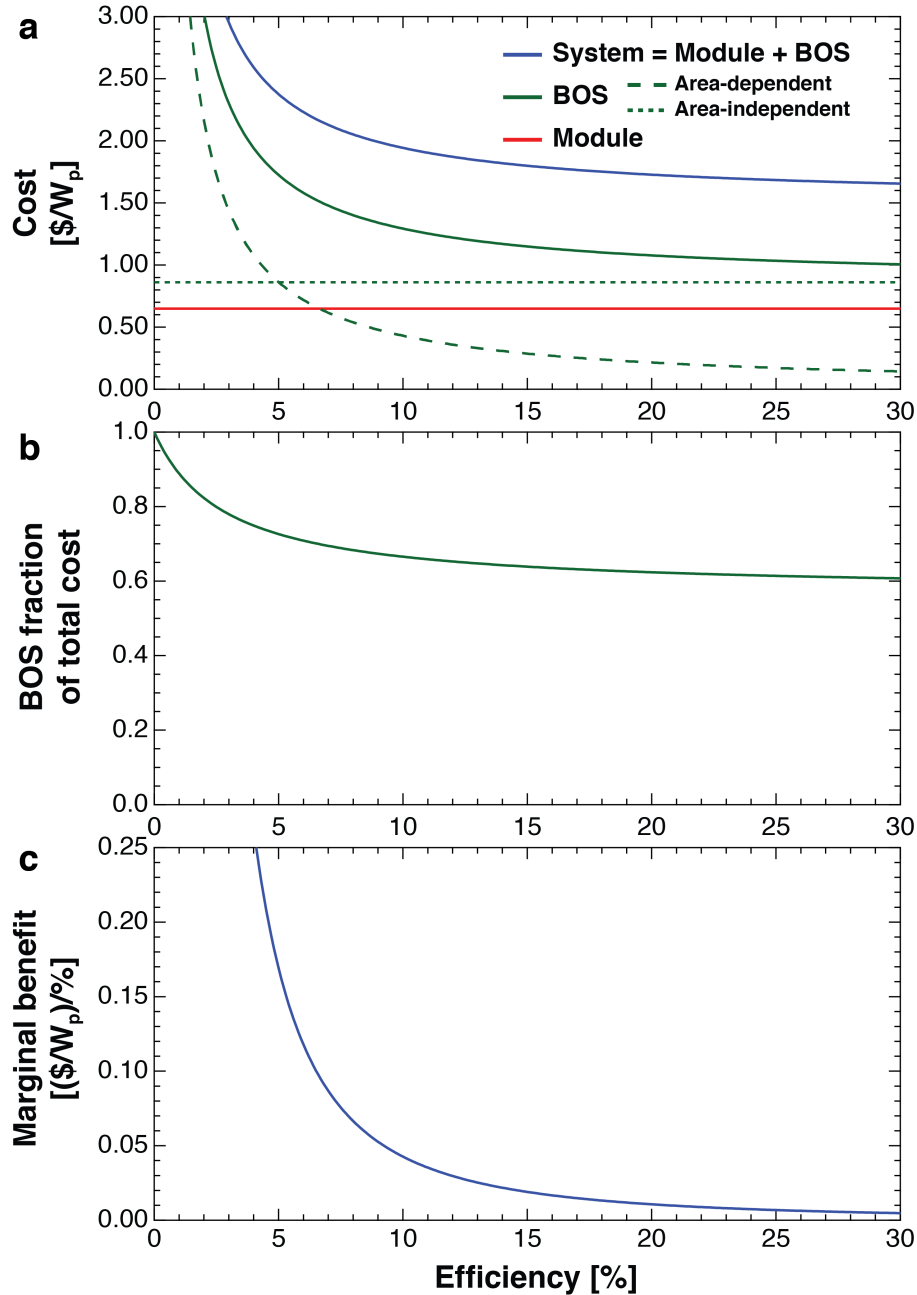
In addition to PV modules, a typical solar PV system also includes additional *balance-of-system* (BOS) components such as combiner boxes, inverters, transformers, racking, wiring, disconnects, and enclosures. Since most BOS components today vary with application but not with PV technology, we refer the reader to the literature on hardware<sup>39</sup> and non-hardware “soft”<sup>40</sup> BOS costs. In a grid-connected system, inverters and transformers convert the low-voltage *direct-current* (DC) output of a solar array into high-voltage *alternating-current* (AC) power that is fed into the electric grid. In an off-grid system, the DC output may be utilized directly, or batteries and charge controllers may be incorporated to store energy for later use.



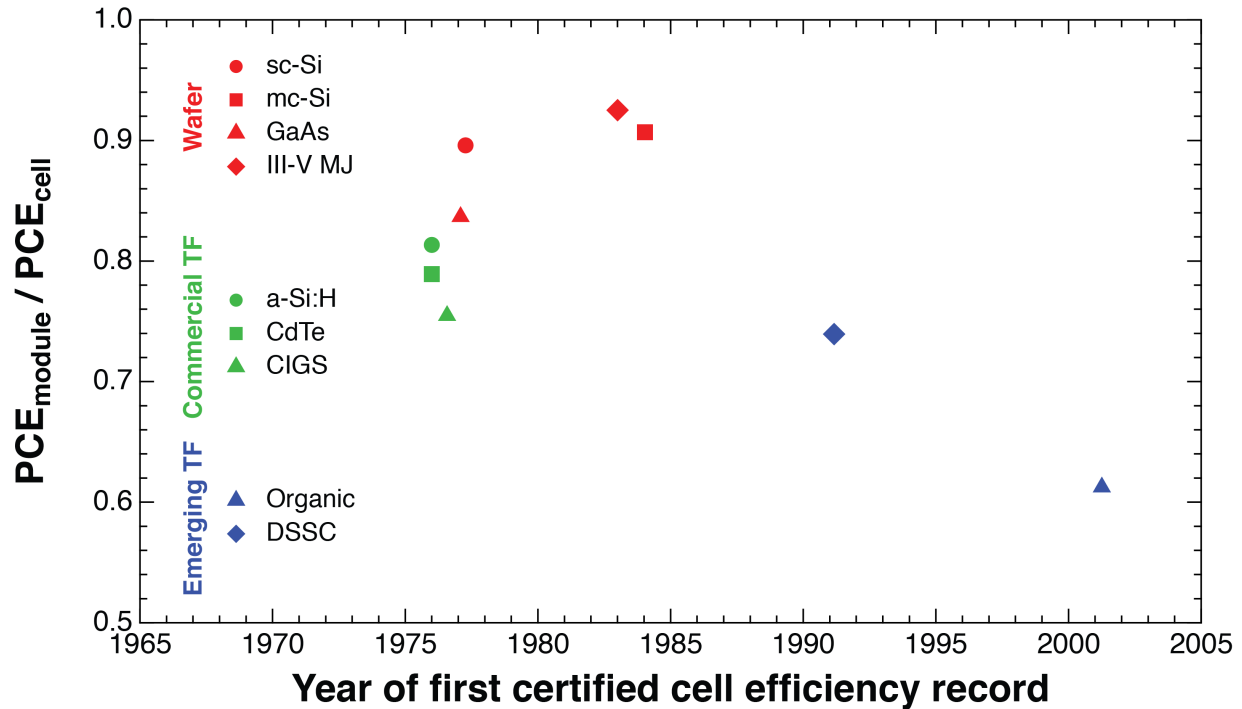
**Fig. S9:** Schematic representation of a solar cell, a solar PV module incorporating multiple cells, and a solar PV array incorporating multiple modules. Balance-of-system components such as racking, wiring, inverters, and transformers are not shown.



**Fig. S10:** (a) Illustration of grid-connected PV system. (b) Breakout view of PV module.



**Fig. S11:** Effect of module efficiency on PV system cost. (a) Contribution of module and BOS to system costs. BOS cost components can be divided into two categories: area-dependent (e.g., land, materials and labor for wiring and mounting) and area-independent (e.g., inverters, permitting, interconnection, and taxes). One-quarter of BOS costs at 15% PCE are assumed to scale with area, consistent with estimates for a fixed-tilt utility-scale system.<sup>41</sup> At 15% PCE, modules constitute 36% of the total system cost of  $\$1.80/W_p$ .<sup>29</sup> A constant module price of  $\$0.65/W_p$  is assumed.<sup>42</sup> (b) Higher module efficiencies reduce the importance of area-dependent and hence total BOS costs. At low efficiencies, the fraction of the system cost attributable to BOS approaches unity due to the larger system area required. (c) The marginal cost reduction from increasing PCE by a fixed quantity (e.g., one percentage point) decreases with increasing absolute efficiency.



**Fig. S12:** Effect of development time on relative record efficiencies of cells and modules. Module efficiencies tend to be closer to cell efficiencies for older technologies. The time elapsed since the first NREL-recognized cell efficiency is used as a proxy for development time.<sup>43,44</sup> We note that this metric is an imperfect proxy, particularly for older technologies. The advent of some solar technologies predates their first certified efficiency measurement; for example, the first modern c-Si cell was demonstrated in 1954, while the first certification reported by NREL occurred in 1977. Early technologies are thus shifted to the right of their true values. Correcting for this effect would likely only strengthen the observed trend. Some emerging thin-film technologies (CZTS, perovskites, and QDPV) are omitted because few or no modules have been demonstrated.

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