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Unlocking the potential of carrier-selective contacts: Key insights for designing c-Si solar cells with efficiency beyond 28 %

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ABSTRACT

Crystalline silicon (c-Si) solar cells are rapidly establishing new efficiency frontiers, with front/back-contacted (FBC) designs now exceeding 26.8 % power conversion efficiency (PCE) and interdigitated back-contacted (IBC) cells surger limitepassing 27 %. This progress is driving a shift from traditional FBC PERC architectures to high-performance TOPCon, SHJ, and IBC configurations, with carrier-selective contacts (CSCs) at the core of these breakthroughs. In this work, we identify three critical factors underpinning CSC effectiveness: the work function of contact layers, energy barriers at heterointerfaces, and energy alignment across the stack of layers forming the CSC. By using advanced numerical simulations, we establish a framework for evaluating and optimizing CSC designs, including state-of-the-art poly-Si, SHJ, and dopant-free structures. We also introduce novel architectures based on TCO materials with potentially simpler manufacturing processes. Our simulations reveal that advanced FBC structures, can reach PCEs up to 28 % deploying localized CSCs architecture. In optimized IBC configurations, efficiencies as high as 28.64 % are achievable. For both, FBC and IBC configurations patterning limitations remain a barrier to theoretical efficiency peaks. Future advances in precision patterning could further close this gap, pushing c-Si solar cells closer to their intrinsic limits. This study provides a roadmap for high-efficiency CSC integration in next-generation c-Si solar cells, establishing pathways to achieve performance over 28 % and accelerating the evolution of photovoltaic technology.

1. Introduction

Recent progresses in crystalline silicon (c-Si) solar cell technologies have set new efficiency records, with top manufacturers achieving certified power conversion efficiencies (PCE) exceeding 26.8 % for front/back-contacted (FBC) architectures based on poly-silicon (poly-Si) and silicon heterojunction (SHJ) designs [1,2]. Additionally, interdigitated back-contacted (IBC) solar cells have demonstrated certified PCEs exceeding 27 % at the cell level [3,4], with module-level efficiencies surpassing 25 % [5]. These trends clearly evidence the strong interest in research and development for high-efficiency c-Si solar cells.

As a result, the prevailing PERC (Passivated Emitter and Rear Cell) architecture, which has long dominated the photovoltaic (PV) market, is expected to cede ground to advanced FBC industrial TOPCon [6] or SHJ architectures, as well as IBC configurations. Further, this market transformation is motivated by the lower capital expenditure (CAPEX) of FBC TOPCon compared to SHJ or IBC counterparts, despite all these architectures exhibiting PCEs nearing 27 % [7].

These efficiency gains are made possible by advancements in modern manufacturing techniques for processing carrier-selective contacts (CSC) together with the exceptional quality of c-Si wafers, bringing solar cells closer to the intrinsic limit [8,9]. Despite approaching the highest attainable theoretical efficiencies, there remains room to push c-Si solar cells beyond 27 % or, possibly, demonstrate even more cost-effective and high-efficiency solar cells architectures. In the longer term, perovskite/c-Si tandem solar cells - already achieving certified efficiencies as high as 34.6 % [10] - are expected to disrupt the market with ongoing rapid research and development. While the industry works to scale and industrialize this tandem technology, there is an urgent need to focus on further optimizing single-junction c-Si architectures. This period of innovation is critical to bridge the gap before tandem solar cell technologies are fully scaled and industrialized. In this context, the exploration and development of novel c-Si solar architectures capable of exceeding 27 % PCE is essential to drive the next wave of high-efficiency solar cell technologies.

In this work, we assess various state-of-the-art CSC designs employed in c-Si solar cells, including poly-Si, SHJ, and dopant-free structures, while introducing novel architectures. By focusing on CSC designs that optimize charge collection and minimize recombination, we address key efficiency drivers. Through advanced numerical simulations, we investigate different solar cell architectures in both FBC and IBC configurations. Our findings provide a comprehensive understanding of state-ofthe-art solar cells and introduce new CSC structures. Moreover, we propose the pathways for solar cell optimization for efficiencies beyond 27 % or even 28 %, closer to their theoretical efficiency limits. This work provides both a detailed analysis of the mechanisms driving CSC for high

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efficiency and a roadmap for the next generation of high-efficiency solar cells as supporting guidelines for progress in the photovoltaic industry.

2. Carrier-selective contacts (CSC)

Charge carrier separation in solar cells is driven by the electric field established at the front and rear surfaces of the absorbing material. In state-of-the-art c-Si solar cells, so-called carrier-selective contacts, also sometimes referred to as carrier-selective passivating contacts, are responsible for building such electric field and controlling the carriers' population within the device [11,12]. The electric field in c-Si solar cells can be induced by two mechanisms: through ionized dopants or by depositing a material with sufficient built-in potential to induce an energy band bending inside c-Si [13]. In the additive manufacturing process of modern c-Si solar cells, the built-in potential is the difference in work function between the substrate and the deposited material. Ideally, either type of charge carriers accumulates at the appropriate c-Si/CSC interface and eventually reach their respective electrodes. CSC typically consists of heterostructures containing a passivating layer, which chemically passivates defects at the c-Si interface and protects it during subsequent processing. However, these heterostructures introduce interface discontinuities that create energy barriers, which can impact charge collection. Charge transport across these heterointerfaces and over energy barriers occurs via thermionic emission or tunnelling, depending on the characteristics of the barrier and the energy alignment between accumulated carriers and available energy states on either side of the heterointerface [14-18]. Note that, depending on the type of collected charge, the CSC provides selective transport of either electrons or holes, working as an Electron Transport Layer (ETL), which selectively transmits electrons while blocking holes, or a Hole Transport Layer (HTL), which transmits holes while blocking electrons [19]. Accordingly, we note the three key factors that influence the transport of charge carriers through CSCs:

i) The work function (Φ) of deposited layers. The induced electric field in the absorber bulk is a consequence of the built-in potential between deposited layers and the absorber bulk [18]. This electric field bends the semiconductor bulk's energy bands, thereby controlling the carriers' population nearing the c-Si interface [20,21]. The built-in potential, determined by the Fermi energy levels of the isolated absorber bulk and the *isolated* deposited layer plays a fundamental role in defining the type of carriers to be collected, thus determining whether the CSC works as an electron contact by an ETL or a hole contact by a HTL. In this respect, the work function of the deposited layers is crucial to establish the electric field in the absorber bulk [11, 13,22]. With respect to the absorber bulk's work function, a lower work function in the deposited layer designates the layer an ETL, whereas a higher work function defines the layer an HTL. Therefore, the work function of the deposited layer is crucial for the effective operation of CSC. The work function is the minimum energy required to remove an electron from a solid material into a vacuum [23]. Using the vacuum energy (E_{vac}) as the reference with 0 eV, the work function Φ of the *isolated* material is equivalent to the Fermi energy with respect to the vacuum (E_F) :

$$\Phi = E_F - E_{vac} = E_F = f(N_D, \chi, E_g, \rho_{trap}, D, n, p)$$

$$\tag{1}$$

Here, E_F , and thus Φ , depends on properties such as the carrier concentration or doping density (N_D), the electron affinity (χ), bandgap (E_g), trapped charge density (ρ_{trap}), density of states of energy (D) and free charge carriers: electrons (n) or holes (p) [13] of the material. Note that in semiconductor materials, it is possible to modify the Fermi energy and thus the work function through doping or introducing ionized impurities or defects in the semiconductor material [24–27].

ii) The energy barriers at the absorber bulk interface. The transport of charge through the heterointerface is driven by tunneling and thermionic emission mechanisms; both depend on the shape of the energy barriers with respect to Fermi level [16,17,22,28,29]. The energy band offset, the Fermi level and the thickness of deposited layers determine the shape of these barriers [17]. Note that the effect of the energy barrier is less apparent when tunneling masses of the materials setting the barrier up are low, as increased tunneling probability facilitates charge transport through heterointerfaces [16, 30]. We refer to energy level and width of the energy barrier as high/low and thick/thin, respectively. For instance, efficient charge collection occurs when the energy barriers in the conduction or valence bands are low and thin, allowing efficient transport of electrons or holes in the n- or p-contact, respectively. Since CSCs are designed to selectively collect only one type of charge carrier, it is desirable to have *high* and *thick* barriers in the valence or conduction bands at the n- or p-contacts, respectively. These barriers effectively hinder the transport of unwanted charge carriers, enhancing the functionality of CSC [18,22]. The transport of charge through the energy barriers is associated with tunneling mechanisms via the tunnel probability $\Gamma(r_t)$ along the position r as discussed in Ref. [22] and it depends on the electrostatic potential $\psi(r)$ within the deposited layers as follows:

$$\Gamma(\mathbf{r}_t) \sim f\left(\int_0^{\mathbf{r}_t} \left(\sqrt{\pm \left(\psi(\mathbf{r}) - E_f\right)}\right) d\mathbf{r}\right)$$
(2)

Where E_f is the Fermi level and $\psi(r)$ is the electrostatic potential. The integral is evaluated between 0, taking the absorber bulk interface as the reference, and the width of the barrier r_t into the CSC. In Eq. (2), $\psi(r)$ is the solution of the Poisson equation and depends on the dielectric constant (ε), N_D , χ , E_g , ρ_{trap} , D, n and p [13] of the materials involved in the CSC:

$$\psi(\mathbf{r}) \sim f(\varepsilon, N_D, \chi, E_g, \rho_{trap}, D, n, p)$$
 (3)

iii) The energy alignment between occupied and available energy states at both sides of the barrier. The transport of charge in semiconductors occurs towards energy states with a certain probability of being occupied, according to Fermi statistics [13]. Such energy states are mostly in the conduction and valence energy bands. The electric field established in the absorber bulk because of the work function of deposited layers results in charge separation. Thanks to such mechanism, the charge carriers accumulate at the front and rear interfaces of the bulk, shifting the Fermi level closer the conduction or valence band energy with respect to the vacuum level. Therefore, depending on the energy gap between the Fermi level and the conduction/valence energy band, the energy states at the bulk interface are mostly occupied by collecting carriers. Similarly, the availability of energy states is essential for the collection of charge on the other side of the energy barrier. Note that the energy alignment reveals the type of tunneling processes: direct, band-to-band and trap-assisted tunneling.

Overall, the three abovementioned key factors are interdependent and influenced by the resulting charge distribution throughout the heterostructure. For this reason, we can evaluate them by solving the Poisson equation:

$$\nabla \bullet (\varepsilon \nabla \psi) = -q(p-n+N_D) - \rho_{trap} \tag{4}$$

Where p and n are holes and electrons density, N_D is the total doping density which is equivalent to the difference in density of donors and acceptors.

Remarkably, solving the Poisson equation (4) provides critical insights into equations (1)–(3). That is, directly solving the Poisson



Fig. 1. Energy band diagram of carrier-selective contacts based on poly-Si. The n-contact (ETL) stack is on the right-hand side of the figure and the p-contact (HTL) is on the left-hand side. Patterned areas indicate the potential barriers in the conduction band (E_c) and in the valence band (E_v).

equation enables a comprehensive evaluation of CSC structures, emphasizing the three key factors governing their performance. To understand the working principle of a certain CSC structure, it is thus essential to use advanced simulations to solve the Poisson equation. The results are illustrated in the so-called *band diagram* in terms of conduction and valence band energy profile across the heterointerfaces using the Fermi energy level as a reference. From these energy band diagrams, the three key factors influencing an effective CSC become evident. In the following sections, for different technologies applied to c-Si solar cells, we assess such key factors to describe the driving mechanisms behind charge collection. Note, we focus on n-type c-Si bulk and we neglect the effect of potential barriers at semiconductor/metal heterointerfaces.

2.1. Poly-Si-based carrier-selective contacts

Carrier-selective contacts based on poly-Si, also known as *Tunneling Oxide Passivating Contact* (TOPCon) [6,31,32] or *polysilicon-on-oxide* (POLO) [33–36] structures, consist of a stack of SiO_x/poly-Si/metal on top of the c-Si absorber bulk. SiO_x is a dielectric material that provides chemical passivation to the c-Si interface [32,37,38]. Poly-Si layers are highly doped n- or p-type depending on the type of charge to be collected [39–42]. As a result of the high-temperature process, some doping atoms diffuse from the poly-Si layer inside the c-Si bulk [43]. Besides, the high-temperature process can also eventually lead to the formation of the so-called pin holes in the ultra-thin SiO_x layer [44–47]. Fig. 1 shows the energy band diagram resulting from the solution of the Poisson equation.

2.1.1. ETL (n-contact)

 The work function of poly-Si n-type depends strongly on the active doping in the poly-Si layer. Low work function values are attained for higher doping values even degenerating the poly-Si material [48–50]. As Fig. 1 depicts, for the n-contact, the higher doping level at poly-Si lead to lower work function with the Fermi energy within the conduction band energy. Note that the electronic properties of poly-Si are very similar to those in c-Si. The work function of this type of layer can be also tweaked by alloying silicon with oxygen or carbon, forming poly-SiO_x [40,51–53] or poly-SiC_x [20,54–57] respectively. These materials respond to the need to realize more transparent CSC compared to poly-Si [58, 59], especially for usage in FBC architectures [60]. Both $poly-SiO_x$ and $poly-SiC_x$, exhibiting wider band gap than poly-Si, can realize a more transparent contact than one based on poly-Si for the same thickness and induce a stronger band bending across the c-Si/SiO_x/poly-Si(O_x)(C_x) heterostructure. However, as doping confinement and related activation in these Si-alloyed layers can be challenging [53,61] and their thickness is kept to a fraction of the poly-Si for exploiting more their optical advantage, such layers are often coated with a transparent conductive oxide (TCO) to support lateral conductivity at the device level [52,54,57,62]. Despite the work function tuneability of such Si-alloyed materials, we note that the working principle for charge transport is the same as in the standard poly-Si, for which, in remainder of this paper, we shall keep the focus on poly-Si only.

- ii) The energy barriers depend in this technology on the properties of the wide bandgap SiO_x material. The energy barriers are illustrated in Fig. 1 as the energy bands difference between c-Si and SiO_x. The height of the potential barrier related to the conduction and valence band offsets is 3.2 eV and 4.7 eV, respectively. The width of the energy barrier is defined by the thickness of the SiO_x layer. From the perspective of electrons from the c-Si bulk, thinner SiO_x layers facilitates their transport. However, the width of the energy barrier for non-collected holes depends also on the thickness of SiO_x layer. In fact, the energy barrier controlled by SiOx controls two competitive conditions: thinner in favor of electron transport and thicker for blocking non-collecting holes. Therefore, we point out that the potential barrier built by SiO_x is crucial not only for passivating the c-Si interfaces, but also for favoring the transport of electrons while blocking that of holes. Note that the presence of generated holes in the defective poly-Si or poly-Si/metal interface enables recombination and the subsequent loss of collecting charge. It is worth noting that the uniformity of SiO_x layers depends on the processing methods and conditions. Furthermore, the pinholes formed in SiO_x during high-temperature process [44,45,47,63] can also impact the transport of charge. Nevertheless, for the purposes of this work, we assume an equivalent uniform SiOx thickness based on references [64,65]. This assumption still considers the transport mechanisms via pinholes, where pinholes may mimic tunneling effects, and vice versa, as detailed in Ref. [66].
- iii) The energy alignment between conduction band energy at the c-Si interface with poly-Si strongly depends on the active doping at



Fig. 2. Energy band diagram of carrier-selective contacts based on SHJ. The n-contact (ETL) is on the right-hand side and p-contact (HTL) on left-hand side. Patterned areas indicate the potential barriers in the conduction band (E_C) and in the valence band (E_V).

the c-Si/SiO_x interface and in the poly-Si layer [29,64,67]. Looking at c-Si/SiO_x and SiO_x/poly-Si interfaces in Fig. 1, we observe that the conduction band energy is aligned at both sides of the barrier. Moreover, the Fermi energy within the conduction band indicates that almost all energy states are aligned for the transport of electrons. It is worth noting that for this structure, the support of the buried dopants inside the c-Si bulk is crucial for the energy alignment because the built-in potential between heavily doped poly-Si and the c-Si bulk is insufficient for achieving the proper alignment of conduction band energy [29,64,65]. The doping level at the c-Si/SiO_x interface is essential for achieving proper energy alignment but note that high doping levels in the absorber bulk increase intrinsic recombination losses. In this regard, ref. [64] reports optimal doping profiles to achieve energy band alignment while minimizing the impact of intrinsic recombination.

Looking at the three key factors together, we note that the carrier collection and energy alignment enable electron transport along the conduction band. The transport processes are based on tunnelling mechanism combined with current flow via pinholes [36,68,69].

2.1.2. HTL (p-contact)

Fig. 1 shows that the p-contact exhibits similar energy variations and barrier shapes to those of the n-contact case but from the perspective of collecting holes along the valence band energy. Therefore, for p-contact based on poly-Si CSC, the working principle is similar to that of n-contact poly-Si CSC [64] as well as $poly-SiO_x$ [40] or $poly-SiC_x$ [54]. The work function of the p-type poly-Si depends on Boron ionized doping. The energy barriers are similar to the n-contact but from the perspective of collecting holes and blocking non-collecting electrons. The energy alignment account for similar conditions and approaches to n-contact but along the valence band. Hence, after the evaluating the three key factors, similar transport as the n-contact is attained but from the perspective of valence band energy and hole as charge carrier.

2.2. Silicon heterojunction (SHJ) carrier-selective contacts

CSC based on SHJ consist of a stack of thin-film silicon layers deposited on top of a c-Si bulk [11,70,71]. The layers forming the contact are a hydrogenated intrinsic amorphous silicon (i-a-Si:H) layer, a doped thin-film layer, a transparent conductive oxide (TCO) layer and a metal layer [72–75]. The role of i-a-Si:H is to passivate the c-Si dangling

bonds at the interfaces and therefore mitigating surface recombination [76,77]. The electronic properties of i-a-Si:H are strongly determined by the arrangement of silicon and hydrogen atoms, mostly exhibiting a bandgap of around 1.7 eV [77]. Doped thin-film silicon layers are deposited on top of the i-a-Si:H and their role is to induce an electric field in favor of collecting charge carriers: electrons for n-contact and holes for p-contact. The electronic properties of such doped layers can be tuned depending on the composition of precursors (e.g. containing C, O, H atoms) and their material phase, since they can exhibit multi-phase composition due to nanocrystals embedded in an amorphous phase [78-87]. For the sake of simplicity, in this work, we consider doped layers with 1.7 eV bandgap. TCO materials are oxides endowed with certain compounds which act as dopants. The role of the TCO layer is twofold: to protect thin-film silicon layers from subsequent processes and the environment, and to support the lateral transport of carriers. In this work, we use indium-tin-oxide (ITO) as baseline TCO in SHJ CSC. Note that in this structure, we have two heterointerfaces: c-Si/i-a-Si:H and doped thin-film layer/TCO [30].

2.2.1. ETL (n-contact)

i) The work function of the n-type thin film, named here n-layer, depends on its active doping and electron affinity γ . In general, higher doping shifts the Fermi energy towards the conduction band energy with respect to the vacuum level. Similar to the abovementioned poly-Si case, the electron affinity χ of a-Si:H layers can be tuned by adding additional compounds to the lattice such as oxygen [87,88] or carbon [89-91]. To enable such an incorporation, deposition regimes typically result in so-called nano-crystalline silicon-oxide [78,80,81,85,87,92–94] or silicon-carbide [57,90,95,96] (nc-SiO_x:H or nc-SiC_x:H) which accommodate also better doping [97,98], resulting in higher conductivity than a-SiH counterpart layers. As their bandgap increases with respect to a-Si:H, they have proven to be a game changer in obtaining very high short-circuit current density (Jsc) while still realizing excellent open-circuit voltages (Voc). Stacking different n-type a-Si:H and/or nc-Si(Ox)(Cx):H layers attains to the domain of surface engineering and contact stack opto-electrical optimization [1,22,72]. In the context of this physical explanation, the doping in the n-layer is directly linked to the activation energy (E_a) . Similarly, TCO layers with low work function eventually support the induced electric field along the contact [22]. The lower the activation energy of an n-layer, the



Fig. 3. Energy band diagram of carrier-selective contacts based on TMOs. The n-contact (ETL) is on the right-hand side and p-contact (HTL) on left-hand side. Patterned areas indicate the potential barriers in the conduction band (E_C) and in the valence band (E_V).

lower the work function is. In Fig. 2, we observe that the $E_{a,n}$ is represented as the energy between the Fermi Energy and the conduction band energy in the n-layer. The work function on TCOs is controlled by the carrier doping concentration. In fact, the higher the carrier concentration is, the lower the TCO work function is [22,24,30].

- ii) The energy barriers for electrons originate from the c-Si/i-a-Si:H interface up to the n-layer/TCO interface. The height of the barrier is related to the band offset at those interfaces. The energy band offset in the conduction band is around 0.1 eV and 0.8 eV at the c-Si/i-a-Si:H and n-layer/TCO interface, respectively. The width of the barrier depends mainly on the combined thickness of the i-a-Si:H and n-type layers. The shape of the energy barrier strongly depends on the $E_{a,n}$ in the n-layer as shown in Fig. 2. Low E_a values reduce the area of the energy barrier for electrons [22] (note the dashed area in Fig. 2). The energy barrier for non-collected holes is formed by the combination of i-a-Si:H, n-layer and TCO layers, resulting in a potential barrier for holes larger than that for electrons. In this regard, the holes face an energy barrier higher than the TCO bandgap, due to the energy difference between the valence band and the Fermi level. This is ascribed to the fact that TCO is commonly a degenerate n-type material, where the Fermi level surpasses the conduction band, thus increasing the barrier for hole transport (see Fig. 2).
- iii) *The energy alignment* occurs along the conduction band energy considering the energy barrier for electrons (see the Fermi energy at the n-contact in Fig. 2). At the c-Si/i-a-Si:H interface accumulated electrons occupying energy states are energetically aligned with available energy states in the TCO. The population of electrons at c-Si/i-a-Si:H interface is controlled by $E_{a,n}$ in the n-layer and the available energy states for electrons in the TCO is determined by its carriers' concentration (N_{TCO}) [30].

These three factors concurrently reveal that the transport occurs through the conduction band enabling direct energy transition processes such as thermionic emission or direct tunnelling as discussed in Refs. [30,99].

2.2.2. HTL (p-contact)

 The work function of p-type thin film, named here p-layer, depends on the active doping in the p-layer and the valence band energy with respect to the vacuum energy. Here, the *E_{a,p}* is the energy gap between the Fermi energy and the valence band energy as Fig. 2 illustrates. In this case, higher doping enables higher work function by shifting the Fermi energy towards the valence band energy with respect to the vacuum level. The valence band energy with respect to the vacuum is the summation of the electron affinity χ and bandgap E_g , both parameters are tunable, like in case of the n-layer, by adding additional elements to the lattice such as oxygen or carbon. TCO layers with high work function eventually support the induced electric field along the contact [22,100]. Note that lower carrier concentration in the TCO eventually results in a higher work function [24].

- ii) The energy barrier for holes arises from the c-Si/i-a-Si:H interface up to the p-layer/TCO interface. The shape of the barrier depends on 0.6 eV band offset at c-Si/i-a-Si:H interface and the $E_{a,p}$ of the p-layer, as Fig. 2 illustrates. The width of the barrier is based on the combined thicknesses of the i-a-Si:H layer and p-layer. Interestingly, at p-layer/TCO interface, the barrier at the valence band energy is 3.7 eV. Note TCO is an n-type degenerated semiconductor which rejects the presence of holes. Therefore, the transport of positive charge towards the TCO material happens via the flow of electrons in TCO towards the p-layer as explained later when we analyze the energy alignment. The energy barrier for electrons is built by both the i-a-Si:H layer and p-layer. The shape of the barrier at the conduction band energy strongly depends on the $E_{a,p}$ and the bandgap of the p-layer [22]. Lower $E_{a,p}$ values increase the potential barrier for non-collecting electrons.
- iii) *The energy alignment* occurs between holes occupying energy states at the c-Si/i-a-Si:H interface and the available energy states on TCO. The energy alignment of energy states is illustrated in Fig. 2 by the Fermi energy across the p-contact stack. Available energy states for holes at c-Si/i-a-Si:H interface depend mostly on the $E_{a,p}$ of the p-layer. The available energy states at TCO are in the conduction band for electrons and depend on TCO carriers' concentration (N_{TCO}). Note that energy alignment here occurs via valence band energy at the c-Si/i-a-Si:H interface and conduction band energy in the TCO layer.

These three factors indicate together that the positive charge transfer occurs by holes transport in the valence band energy at c-Si/i-a-Si:H and p-layer. At the p-layer/TCO interface, the energy intra-band energy alignment enables band-to-band tunneling processes or trap-assisted tunneling if using energy states within the bandgap of p-layer as discussed in Ref. [30]. We note therefore that the usage of TCO layers in

both ETL and HTL SHJ CSCs has far reaching implications than merely boosting the optical performance of SHJ solar cells as previously thought, especially looking at the rear side of a monofacial device to limit parasitic absorption in the metallic contact [101,102].

2.3. Carrier-selective contacts based on transition metal oxides (TMO)

The use of TMOs becomes attractive due to their relatively low absorption combined with the tunable electronic properties such as the work function. Such materials are good candidates to replace the Sibased doped layers in SHJ solar cells depending on their work function [11,26,27,103–105]. Due to that specific reason, c-Si solar cells endowed with such materials are typically dubbed *dopant-free* designs [11,105–112], even though doping is still present inside the bulk, at least. In this work, due to the promising opto-electronic properties and feasibility, we use TiO_x and MoO_x as ETL and HTL representatives, respectively [25,113–119]. Additionally, we use ITO and IWO as TCOs on top of ETL and HTL, respectively. In principle, TiO_x and MoO_x can replace Si-based doped thin-film layers in SHJ stacks. For this reason, we use a baseline structure with i-a-Si:H passivating layer like SHJ CSC. The resulting energy band diagram is depicted in Fig. 3 with ETL (TiO_x) on the right-hand side and HTL (MoO_x) on left-hand side.

2.3.1. ETL (TiO_x)

- i) *The work function* of TiO_x, ITO and c-Si are calculated to be 4.15 [120], 3.8 [24] and 4.24 eV, respectively (see Table 2). The work function of both TiO_x and ITO are lower than the work function of the c-Si bulk. Therefore, the combination of both materials induces the electric field at the c-Si interface attracting electrons towards the c-Si/i-a-Si:H interface. We note that the work function of TiO_x is only about 0.1 eV smaller than that of c-Si bulk, enabling a limited electric field in c-Si. For this reason, we tuned the work function of ITO to 3.8 eV by increasing the N_{TCO} to 5 × 10^{20} cm⁻³ [24]. The resulting electric field of these layers becomes evident as the band bending in c-Si in Fig. 3.
- iv) The energy barrier for electrons in the conduction band energy is formed from the c-Si/i-a-Si:H interface up to the TiOx/ITO interface. The width of the barrier is the sum of the thicknesses of the i-aSi:H and TiO_x layers. The shape of the potential barrier for electrons is affected by the band offset of the c-Si/i-a-Si:H and i-a-Si:H/TiO_x interfaces, which are relatively small and in the order of 0.1 eV. Additionally, the work function in each layer affects the shape of the energy barrier. In this regard, lower work function values on subsequent layers of the heterostructure reduce the area of the energy barrier for electrons. Like the n-contact in the SHJ CSC case, the energy barrier for non-collected holes is formed by the i-a-Si:H, TiO_x, and TCO layers. The potential barrier for holes is larger than that for electrons, as TiO_x behaves like an n-type material in addition to the contribution of ITO material. The resulting potential barriers are depicted in Fig. 3 as patterned areas.
- ii) *The energy alignment* occurs on the conduction band energy (see the Fermi energy at ETL in Fig. 3). The energy states for accumulated electrons at the c-Si/i-aSi interface are energetically aligned with available energy states at the TiO_x/TTO interface. The energy states available for electrons at c-Si/i-a-Si:H interface are mainly affected by the work function of TiO_x and the available energy states for electrons on ITO are determined by the doped carrier concentration N_{TCO} .

These three factors point together at a transport like the one described in case of n-contact in SHJ CSC. That is, the transport of electrons occurs via electrons towards the conduction energy band [105], enabling direct energy transition processes such as thermionic emission or direct tunnelling [30].

2.3.2. HTL (MoO_x)

- i) The work function of MoO_x , IWO and c-Si are calculated to be 6.2 eV, 4.4 and 4.24 eV, respectively (see Table 2). Specifically, the work function value for the IWO TCO is related to $N_{TCO} = 1 \times 10^{20}$ cm⁻³. Both MoO_x and IWO layers exhibit higher work function than that of c-Si bulk. This allows to induce an electric field in c-Si and to accumulate holes at the c-Si/i-a-Si:H interface by bending the valence band energy towards the Fermi energy as we observe in Fig. 3.
- ii) The energy barrier for holes is formed by two sections: from the c-Si/i-a-Si:H up to the i-a-Si:H/MoO_x interface and from the i-a-Si: H/MoO_x interface towards MoO_x and IWO layers. The width of such a barrier is inherent to the thickness of the i-a-Si:H layer in the first section. The band offset at the c-Si/i-a-Si:H interface (0.6 eV) and the work function of MoO_x controls the shape of the potential barrier. The area of the barrier is relatively small thanks to the 6.2 eV work function of MoO_x as Fig. 3 illustrates. The barrier for holes is relatively high with values up to 3.7 eV like the case of p-contact in the SHJ CSC case. Here, MoOr and IWO are degenerate n-type materials blocking the transport of holes. Accordingly, the transport of positive charge through MoO_r and IWO occurs via the flow of electrons from IWO towards the i-a-Si: H. At the i-a-Si:H/MoO_x heterointerface, the conduction band energy of the MoO^x layer merges with the valence band energy of the i-a-Si:H. Such a condition is due to the assumption of theoretically perfect materials discontinuity. In reality, it is worth noting that such large discontinuity leads to the formation of a dipole as discussed in Refs. [25,119]. In this work, for the sake of simplicity, we assume perfect discontinuities at heterointerfaces to calculate the energy band diagram as depicted in Fig. 3. The energy barrier for electrons is formed only by the i-a-Si:H layer. The shape of the barrier at the conduction band energy strongly depends on the work function of MoOx and the c-Si/i-a-Si:H band offset of 0.1 eV. It is worth noting that the barrier of electrons here is relatively small depending on the i-a-Si:H layer and MoO_x work function. Therefore, it is crucial for MoO_x to experimentally achieve high work function [25,119].
- iii) The energy alignment occurs between holes occupying energy states at the c-Si/i-a-Si:H interface and the available energy states for electrons at the i-a-Si:H/MoO_x interface as well as in the conduction band energy of both MoO_x and IWO layers. The Fermi energy crossing the HTL contact in Fig. 3 illustrates the alignment of energy states. Available energy states for holes at c-Si/i-a-Si:H interface depend on the work function of MoOx. The available energy states for electrons at the i-a-Si:H/MoO_x interface as well as in the MoO_x and IWO layers are in the conduction energy band. These energy states are affected by the carrier concentration in both MoO_x and IWO layers. However, the carrier concentration in IWO has a more pronounced impact on determining the available energy states due to its electronic properties. Like in the case of Si-based p-contact SHJ CSC, the energy alignment occurs via valence band energy at c-Si/i-a-Si:H interface and the conduction band energy at the i-a-Si:H/MoOx interface as well as MoOx and IWO layers. The core of the energy alignment is the Fermi energy in or the work function of the MoO_x layer. Thus, the work function of MoO_x and the energy transition at i-a-Si:H/MoO_x heterointerface are essential for the proper energy alignment [25,118].

These three factors together expose that, much like in the case of pcontact in SHJ CSC, the positive charge transfer occurs by the transport of holes in the valence band energy through the c-Si/i-a-Si:H interface and i-a-Si:H layer. At the i-a-Si:H/MoO_x interface, the alignment of the valence band of the i-a-Si:H layer and the conduction band energy of the MoO_x enables band-to-band or trap-assisted-tunneling if using energy states within the bandgap of i-a-Si:H as discussed in Refs. [30,118]. It is



Distance, r

Fig. 4. Energy band diagram of carrier-selective contacts based on TCOs. The n-contact (ETL) is based on AZO (right-hand side) and p-contact (HTL) is based on IWO (left-hand side). Continuous lines indicate energy bands using $N_{TCO-IWO} = 1 \times 10^{19}$ cm⁻³ and dashed lines energy bands using $N_{TCO-IWO} = 1 \times 10^{20}$ cm⁻³ in HTL IWO. Patterned areas indicate the potential barriers in the conduction band (E_C) and in the valence band (E_V) for a structure featuring $N_{TCO-IWO} = 1 \times 10^{19}$ cm⁻³.

worth mentioning the crucial role of the work function of MOO_x in achieving a functional HTL CSC. Moreover, both interfaces around the MOO_x layer exhibit relatively high energy discontinuities, especially at the i-a-Si:H/MOO_x interface. Such discontinuities indicate the properties to look for in the deposited MOO_x thus setting the origin of interface mechanisms at i-a-Si:H/MOO_x as reported in Refs. [25,27,119,121].

2.4. TCO-selective CSC

Looking at SHJ and TMO structures, we observe that negative and positive charge collection at TCO is based only on electrons. For negative charge transport, the flow of electrons occurs on the way from c-Si towards the metal electrodes and, for positive charge transport, the flow of electrons is reversed. Moreover, typical TCOs are degenerated n-type semiconductors inherently blocking the flow of holes. In Ref. [72], we propose a novel solar cell structure which exploits such features of TCO. In this section, we explain the working principle of the so-called *TCO selective* CSC. The contact stack is based solely on TCOs with the proper work function on top of the i-a-Si:H passivating layer to act as an ETL or HTL layer. In this regard, we use AZO [24] and IWO [122,123] to build the ETL and HTL, respectively. We calculate the energy band diagram and report it in Fig. 4.

2.4.1. ETL (AZO)

- i) The work function of AZO is 3.4 eV [24]. Such a value is enough to induce a band bending in c-Si, attracting electrons to the c-Si/i-a-Si:H interface, as Fig. 4 depicts. To achieve 3.4 eV work function on AZO, we use a carrier concentration value of 5×10^{20} cm⁻³ in our calculations.
- ii) *The energy barrier for electrons* is like ETL in Section 2.3.1. The energy barrier goes from the c-Si/i-a-Si:H interface to the i-a-Si: H/AZO interface. The width of the barrier depends on the thickness of the i-a-Si:H layer. The shape of the energy barrier is tuned by the work function of AZO together with the 0.1 eV band offset at the c-Si/i-a-Si:H interface. From the perspective of electrons, a lower work function in AZO reduces the area of the barrier in the conduction band energy. *The energy barrier for holes* starts at the c-Si/i-a-Si:H interface and includes the AZO layer. AZO, like most TCOs, is a degenerated n-type semiconductor, reducing to almost zero the probability of energy states available

for holes as the Fermi energy is energetically far from the valence band.

iii) *The energy alignment* appears on the conduction band energy (see the Fermi energy at ETL in Fig. 4). The energy states for electrons at the c-Si/i-a-Si:H interface are aligned with available energy states at the i-a-Si:H/AZO interface. The amount of energy states available for electrons at the c-Si/i-a-Si:H interface depends only on the work function of AZO, and the carrier concentration N_{TCO} in AZO defines the quantity of available energy states for electrons in AZO.

These three factors highlight the fact that the transport of negative charge occurs via electrons along the conduction energy band enabling direct energy transition processes such as thermionic emission or direct tunneling, like the case of ETLs in SHJ and TMO CSC contacts. However, it is worth mentioning that achieving low work function with AZO (TCO) is crucial for the proper working mechanisms of this structure.

2.4.2. HTL (IWO)

- i) The work function of IWO is 5.4 eV. To achieve such a value, we use as reference an IWO with work function value of 5.2 eV with an N_{TCO} of 1×10^{20} cm⁻³ [122]. In our calculations, we assume 1×10^{19} cm⁻³ carrier concentration to get a work function of 5.4 eV. The effect on the energy bands of IWO with 1×10^{20} cm⁻³ and a work function of 5.2 eV, compared with the case of 1×10^{19} cm⁻³ and a work function of 5.4 eV, is illustrated in Fig. 4. We note that the IWO with a work function of 5.4 eV provides a more favorable band bending for holes.
- ii) The energy barriers for holes and non-collecting electrons are like those in the case of TMO CSC (see section 2.3.2). The features of the energy barrier for holes and electrons, like thickness and shape, depend on the i-a-Si:H layer thickness and the work function of IWO. IWO, like most of TCOs, is an n-type degenerated material blocking holes. Like in the case of MOO_x CSC, the conduction band energy of the IWO merges with the valence band energy of the i-a-Si:H layer at i-a-Si:H/IWO interface. Therefore, similar observations made in section 2.3.2 can be applied to this structure. In this case, it is worth noting that there are no empirical observations of interface phenomenon for this structure yet. Nevertheless, in this work, we assume perfect discontinuities at heterointerfaces to calculate the energy band diagram depicted

Different carrier-selective contact materials and parameters controlling th	e three key factors: work function,	energy barriers and energy alignment.
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CSC			Key factors		
	Charge Transport	Material	Work Function	Energy Barriers	Energy Alignment
Poly-Si	ETL	n-type poly-Si	Doping	d _{ox}	Doping
	HTL	p-type poly-Si	Doping	d_{ox}	Doping
SHJ	ETL	n-type a/nc-Si:H	Ea	E_a, Φ_{TCO}	E_a, N_{TCO}
	HTL	p-type a/nc-Si:H	Ea	E_a, Φ_{TCO}	E_a, N_{TCO}
ТМО	ETL	TiO _x	Φ_{TiO_x}	Φ_{TiO_x}, Φ_{TCO}	Φ_{TiO_x}, N_{TCO}
	HTL	MoO _x	Φ_{MoO_x}	Φ_{MoO_x}, Φ_{TCO}	Φ_{MoO_x}, N_{TCO}
TCO	ETL	AZO	Φ_{AZO}	Φ_{AZO}	Φ_{AZO}, N_{AZO}
	HTL	IWO	Φ_{IWO}	Φ_{IWO}	Φ_{IWO}, N_{IWO}
TCO with Si-in-diffusion	ETL	n-type c-Si	Doping	Φ_{TCO}	Doping, N _{TCO}
	HTL	p-type c-Si	Doping	Φ_{TCO}	Doping, N_{TCO}

in Fig. 4. We point out that the shape of the energy barrier for electrons is relatively small and very sensitive to the work function of IWO.

iii) The energy alignment occurs between energy states for holes at the c-Si/i-a-Si:H interface and energy states for electrons at the i-a-Si: H/IWO interface (see the Fermi energy across the HTL in Fig. 4). The number of available energy states for holes at the c-Si/i-a-Si: H interface depends on the work function of IWO. The amount of available energy states for electrons at i-a-Si:H/IWO interface and in IWO depends on the carrier concentration of IWO. The core of the energy alignment stands on the Fermi energy of IWO. Therefore, the work function of IWO is critical for the proper energy alignment.

These three factors together reveal that the positive charge transfer occurs in the valence band energy at the c-Si/i-a-Si:H interface and in the i-a-Si:H layer. Then, at the i-a-Si:H/IWO interface, the energy alignment between the conduction band energy of the IWO and the valence band energy of the i-a-Si:H enables band-to-band tunneling or trap-assisted-tunneling mechanisms, like in the MoO_x CSC case. Achieving high work function TCO is essential for reaching a functional HTL contact. Similar to the MoO_x CSC case, we anticipate interface phenomena occurring at the i-a-Si:H/IWO interface.

In general, the work function of the TCO layers is pivotal for an effective carriers' extraction in this type of contact stack. Therefore, the reliability of such a structure stands mostly on TCO processing and

limiting possible damages to the passivating layer underneath. To relax the properties of TCOs in this structure, we propose to include a doping profile extending inside the bulk in a novel c-Si solar cell structure, namely a TCO-selective with buried doping [51]. Like in the poly-Si CSC case (see Section 2.1), the doping profile is n-type and p-type for ETL and HTL, respectively. Interestingly, such a buried doping can support the induced electric field inside c-Si while achieving the energy alignment of the contact regardless of the TCO work function.

The development of each structure discussed here faces individual technological challenges related to layers and particular interfaces affecting the working principle of CSC, as the case of SHJ CSC discussed in Ref. [30]. Table 1 summarizes the key properties of the CSC determining an efficient charge collection. Information reported provides insights and guides future research and development in CSC. Note that the three key factors thus far discussed (work function, energy barrier(s) and energy alignment) not only define the working principle of CSC in c-Si solar cells but can be applied also to other photovoltaic technologies, such as perovskite, CIGS, etc., (opto-)electronic devices and advanced diodes.

3. Modelling framework for c-Si solar cell designs beyond state of the art

Recent reports on c-Si technology using CSC [1] demonstrate that performance is approaching the intrinsic limit of silicon. Besides the deployment of optimal CSC stacks, such achievements are possible



Fig. 5. Flowchart of the simulation framework. In the input parameters, ε stands for permittivity, T for temperature, μ for mobility, χ for electron affinity, E_g for band gap, $m_{t(\bullet)}$ for tunnelling mass of electrons or holes, $N_{(\bullet)}$ for carrier density or doping concentration, and DOS for density of states. The input parameters are fed to various physical models and coupled with the semiconductor equations: the Poisson equation (Equation (4) in Section 2) and the continuity equation, where $J_{(\bullet)}$ stands for the current density of electron or holes. Such equations are solved consistently with the Fermi-Dirac statistics, where E, E_F and k_B are energy, Fermi energy, and Boltzmann constant, respectively. The calculated results are represented as energy band diagrams and current density – voltage (J–V) curves.



Fig. 6. Schematic illustrations of solar cell designs beyond state-of-the-art, namely: (a) PERFECT - RJ - DST solar cells [67], (b) dopants free SHJ solar cells, (c) TCO selective SHJ solar cells [134], (d) TCO selective with buried junctions [51], (e) SHJ solar cells with localized contacts [135], (f) IBC with poly-Si, (g) IBC hybrid and (h) IBC with SHJ. PERFECT stands for Passivated Emitter Rear Front Contact; RJ for rear junction; and DST for double side textured.

Summary of models and input material parameters. SRV stands for surface recombination velocity.

Crystalline Silicon (c-Si)					
BandgapSchnarrowing[13]MobilityKla	ienk 6] assen	Intrinsic c density SRV	arrier	9.65 × 10 ⁹ 300 K [137 0.01 cm/s	cm ⁻³ at]
SRH lifetime 40	ms [1]	Resistivity		2Ωcm	
Poly-crystalline Silicon (poly-Si)				
n-contact doping	$1 \times 10^{20} \text{ cm}$	⁻³ p-co	ontact dopin		$10^{20}~{\rm cm}^{-3}$
	SiO _x [64]	i-a-Si:H [<mark>30</mark>]	I SHJ n- [30]	layer S	HJ p-layer 30]
Electron affinity (eV) Band gap (eV)	0.9 9	3.9 1.7	3.9 2	3 1	.9 .8
Electron/hole mobility $(cm^2V^{-1}s^{-1})$		20/4	25/5	2	5/5
Relative permittivity	3.9	11.9	11.9	1	1.9
Electron/hole tunneling	04/	0.1	0.1	0	.1
mass (m_0^*)	0.32		20	- 20 -	20
Effective CB DOS (cm ⁻³)		2×10	$20 2 \times 10^{20}$	20 20	$\times 10^{20}$
Activation energy (meV)		2 × 10	60	0	× 10 ·
DOS energy distribution		DOS di	stribution [3	0]	0
	ITO	MoO _x	TiO _x	IWO	AZO
	[30]	[25]	[127]	[122]	[129]
Electron affinity (eV)	4.9	6.3	4	5.6	4.35
Band gap (eV)	3.1	3	3.1	3.1	3.3
Electron/hole mobility	160/	25/25	$0.2/1 \times$	160/40	18/18
$(cm^2V^{-1}s^{-1})$	40		10^{-3}		
Relative permittivity	4	4.27	46	4	4
Electron/hole tunneling mass (m_0^*)	0.1				
Effective CB DOS (cm ⁻³)	4×10^{18}	$6.8 imes$ 10^{18}	$3 imes 10^{21}$	${\begin{array}{c} 4\times\\ 10^{18} \end{array}}$	4×10^{18}
Effective VB DOS	1.7×10^{19}	7.9 ×	3×10^{21}	1.7×10^{19}	1.7 ×
(cm ⁻³)	1017	10"	1×10^{19}	1019	1019
(cm^{-3})	10^{20}	1×10^{18}	1 × 1019		

owing to excellent quality of nowadays c-Si wafers which have demonstrated SRH lifetimes as high as 40 ms [1]. Therefore, it becomes relevant to explore alternative, high-performance c-Si solar cell designs with less materials usage and simplified processing. In the following, we assess advanced FBC and IBC architectures through numerical simulations. To do that we have built a modelling framework capable of evaluating the abovementioned physical mechanisms and indicating guidelines for achieving highest efficiency. It is important to highlight that we consider high quality c-Si interface passivation with J_0 lower than 1 fA/cm² as reported in Ref. [1], tailored for a surface recombination velocity of 0.01 cm/s.

Fig. 5 illustrates the modelling framework we use to study different solar cell designs. The framework is developed around the finite-element simulation package TCAD Sentaurus [124] coupled with in-house developed GenPro4 [125]. We implement a two-dimensional approach for representing the geometry of the symmetric element of different solar cell designs as sketched in Fig. 6. The input parameters are summarized as follows: physical models and material parameters in Table 2, thickness of supporting layers for FBC designs in Table 3 and for IBC designs in Table 4.

The optical situation inside the solar cells is simulated concurrently using wave and ray optics approaches under AM1.5 G illumination. The resulting optical generation profile, together with various the physical models, is coupled with the semiconductor equations for electrical simulation consistently with Fermi-Dirac statistics. Specifically, to study the charge transport mechanisms at heterointerfaces thermionic and tunneling models are coupled too in the semiconductor equations. The solution of the drift-diffusion model provides the energy band diagram and the characteristic current-density - voltage (J-V) curve. This simulation framework can also provide the spectral response as well as the assessment of loss mechanisms in the simulated devices. It is noteworthy that our simulation approach has been validated against various solar cell designs [1,20,22,25,30,57,58,64,72,119,125–133].

In this study, we focus on analyzing the performance of several solar cell designs as function of different design parameters, such as the pitch of the metal contacts and the c-Si wafer thickness. To align the results with the potential conversion efficiency of each structure, we assumed for an optimal light management in our optical simulations both front and rear textured interfaces, random pyramids featuring 54.7° base angle, and silver as metal contact as well as back reflector. Note that due to the inherent complexity of transport mechanisms at heterointerfaces, our electrical simulations consider the approach of flat interfaces for the electrical solution.

Summary of layers thickness and TCO carrier concentration considered for each FBC architecture. (D)ARC stands for (dual) anti-reflective coating.

	Perfect RJ		Dopants free		Localized contacts	
	ETL	HTL	ETL	HTL	ETL	HTL
SiO _x	1 nm	1 nm				
Poly-Si	15 nm	15 nm				
i-a-Si:H			5 nm	6 nm	5 nm	6 nm
SHJ					8 nm	10 nm
layer						
MoO _x				2 nm		
TiO _x			10 nm			
ITO			50 nm (5 $ imes$ 10 ²⁰ cm ⁻³)		55 nm (2 \times 10 ²⁰ cm ⁻³)	50 nm (2 \times 10 ²⁰ cm ⁻³)
IWO				57 nm (1 $ imes 10^{20}$ cm ⁻³)		
(D)ARC	Front:MgF ₂ (103 nm) + SiN _x (61	Back:MgF ₂ (235	Back: MgF ₂ (259 nm)	Front: MgF ₂ (106	Front:MgF ₂ (103 nm) + SiN _x (61	Back:
	nm)	nm)		nm)	nm)	MgF_2
						(235 nm)
	TCO selective		TCO buried junctions			
	ETL		HTL	ETL		HTL
i-a-Si:H	5 nm		8 nm	5 nm		8 nm
ITO				50 nr	n (5 \times 10 ²⁰ cm ⁻³)	
AZO	$10~\mathrm{nm}~\mathrm{(5} imes10^{20}~\mathrm{cm}$	-3)				
IWO			59 nm (1 \times 10 19 cm $^{-3}$)			59 nm (1 \times 10 ²⁰ cm $^{-3}$)
ARC	Back:MgF ₂ (297 nm))	Front:MgF2 (105 nm)	Back	MgF ₂ (224 nm)	FrontMgF2 (105 nm)

Table 4

Summary of layers thickness and TCO carrier concentration considered for each IBC architecture. DARC stands for dual anti-reflective coating.

	IBC pol	y-Si	IBC-Hybrid		IBC-SHJ	
	ETL	HTL	ETL	HTL	ETL	HTL
SiO _x	1 nm	1 nm	1 nm			
Poly-Si	15	15	15			
	nm	nm	nm			
i-a-Si:H				6 nm	6 nm	6 nm
SHJ				10 nm	10	10
layer					nm	nm
ITO				50 nm ($N_{ITO} = 2 \times 10^{20}$	50 nm	$(N_{ITO} =$
				cm ⁻³)	2×10^{2}	20 cm $^{-3}$)
DARC	Front: 1	MgF ₂	Front: 1	$MgF_2 (103 nm) +$	Front: 1	MgF ₂
	(103 nr	n) +	SiN _x (6	1 nm)	(103 ni	m) +
	SiN _x (6	1 nm)	Back: N	/lgF2 (235 nm)	SiN _x (6	1 nm)
	Back: M	IgF ₂			Back: N	∕lgF₂
	(235 nr	n)			(235 ni	n)

4. Novel c-Si solar cell designs

In Section 2, we highlight the key factors for a stack of materials to work effectively as CSC. In Section 3, we report the parameterization of CSC structures that satisfy those conditions (see Table 2). From the processing perspective, achieving materials exhibiting the appropriate parameters is particularly challenging, especially during the formation of heterointerfaces. In this regard, significant progress is ongoing, showing that c-Si technology is approaching its intrinsic limit [8,139] and is well-positioned to investigate novel solar cell designs [140] with extreme and yet feasible technological design parameters. In the following, we evaluate the performance of both FBC and IBC architectures, as shown in Fig. 6, in terms of *Jsc, Voc*, fill factor (*FF*) and efficiency (η) as function of metallic patterning, c-Si bulk wafer thickness and contact resistivity.

4.1. Front/back-contacted structures

The fundamental limitation of solar cell designs based on FBC architecture is the front metallic contact that shades the solar cell from incoming light. Additionally, the front supporting layers usually exhibit parasitic absorption and cover the entire front surface, further without compromising charge collection, we investigate solar cell designs employing CSC reported in Section 2. In this work we are interested in unveiling the highest possible efficiency, therefore we focus only on monofacial solar cell designs. Using poly-Si CSC (see Section 2.1), the Passivated Emitter Rear/Front ConTact (PERFECT) structure with rear junction (RJ) configuration is the most promising reported [67] (see Fig. 6 (a), PERFECT RJ). This solar cell design exhibits the highly absorptive n-type poly-Si film solely beneath the front metallic contact and has a p-type poly-Si CSC covering the full rear side, providing with the best possible hole collection as only vertical transport is then exploited. Next, we evaluate SHJ solar cells with dopants free CSCs (see Fig. 6 (b), Dopants free) as a viable alternative to replace the parasitically absorptive doped Si-based thin-film layers commonly used in SHJ solar cells. From a similar perspective, to develop a more transparent front contact and simplify the production processing, we explore the TCO selective design [134], featuring the front junction (FJ) configuration. The rationale for the FJ configuration is to position the less absorptive IWO (HTL) at the front side and the more absorptive AZO (ETL) at the back side (see Fig. 6 (c)). We also investigate the TCO selective with buried doping design [51] thus relaxing the requirements for TCO materials (see Fig. 6 (d)). Finally, for optimal light management using the standard SHJ CSC structure discussed in Section 2.2, we investigate a solar cell design with the front n-contact localized solely beneath the front metal contact (see Fig. 6 (e)), here referred to as Localized contacts SHJ solar cell [135,141]. Note that we accounted 10-µm thick front metal finger and, unless stated otherwise, 2 Ω cm bulk resistivity in all simulated structures to be able to compare the results. The simulation domain includes solar cells featuring an interfinger pitch range between 400 and 1600 µm (front metallization) and a c-Si thickness range from 50 to 220 µm. Although some of the narrower pitches and/or thinner bulks might be experimentally challenging, we consider realistic our simulation ranges, given the level of sophistication reached by c-Si PV industry.

constraining the light management. To mitigate such optical limitations

Fig. 7 illustrates the simulation results for *Jsc, Voc, FF* and η of the five FBC architectures under study. For a consistent and visual comparison among different solar cell designs, we present the results using a uniform scale. As previously mentioned, we simulate the symmetric element of the various solar cell designs. This means that in the remainder of this work, included the next section on IBC solar cell designs, we shall report results with respect to half of the pitch.



Fig. 7. Simulated Jsc, Voc, FF and η as a function of half pitch and c-Si thickness for FBC solar cells: TCO-selective, dopant-free, Perfect RJ, localized with SHJ and TCO-selective with buried doping architectures.

Summary of the maximum values of the external parameters of the five FBC architectures under study, alongside the related pairs of front metallization pitch and c-Si bulk thickness. Note such pairs change per each external parameter highlighting how different mechanisms of light management, intrinsic recombination, and lateral carrier transport compete in different solar cell designs. Ultimately, the maximum efficiency accounts for the optimal solution.

	<i>Jsc</i> _{max} [mA/ cm ²]	Voc _{max} [mV]	<i>FF</i> _{max} [%]	η_{\max} [%]
PERFECT RJ	43.38 (Pitch = 1600 μ m d _{c-Si} = 220 μ m)	751 (Pitch = any d_{c-Si} = 50 μ m)	86 % (Pitch = 400 $\mu m \; d_{c\text{-}Si} = 100150 \; \mu m$)	27.05 % (Pitch = 800 μm d _{c-Si} = 160 μm)
Dopants free	42.30 (Pitch = 1600 μ m d _{c-Si} = 220 μ m)	766 (Pitch = any d_{c-Si} = 50 μ m)	87.77 % (Pitch = 400 μ m d _{c-Si} = 50 μ m)	27.16 % (Pitch = $1200 \ \mu m \ d_{c}$. si = 70 μm)
TCO selective	42.33 (Pitch = 1600 μ m d _{c-Si} = 220 μ m)	766 (Pitch = any d_{c-Si} = 50 μ m)	87.44 % (Pitch = 400 μ m d _{c-Si} = 50 μ m)	26.98 % (Pitch = 800 $\mu m d_{c-si} =$ 70 μm)
TCO selective with buried junctions	42.43 (Pitch = 1600 μ m d _{c-Si} = 220 μ m)	749 (Pitch = any d_{c-Si} = 50 μ m)	85.6 % (Pitch = 400 μm d _{c-Si} = 100–150 μm)	26.31 % (Pitch = 800 $\mu m d_{c-Si} =$ 190 μm)
Localized contacts	43.38 (Pitch = $1600 \ \mu m$ $d_{c-Si} = 220 \ \mu m$)	766.4 (Pitch = any $d_{c-Si} = 50$ µm)	87.29 % (Pitch = 400 μ m d _{c-Si} = 50 μ m)	27.78 (Pitch = 800 $\mu m \; d_c. _{Si} = 60 \; \mu m)$

Looking at the Jsc contour plots, we note how the Jsc is dominated by larger half-pitch values, which indicate lower front shadowing, and thicker c-Si absorbers, which increase light absorption [8,19,21,142]. In Table 5 we report the maximum Jsc values for the five investigated solar cell designs. The maximum value for each structure, as anticipated, is achieved with solar cells featuring 800 µm half-pitch and 220-µm thick c-Si bulk, which are the maximal values in our simulation domain. We observe that structures with the front surface covered only with ARC layers, such as PERFECT RJ and Localized contacts, exhibit the highest Jsc_{max} values. At the same time, the TCO selective with buried junctions solar cell shows 0.1 mA/cm² improvement as compared to TCO selective solar cell, which can be ascribed to the use of more transparent/reflective TCO on the rear side, which enhances light management. Specifically, the TCO selective solar cell uses AZO on the rear side that is more absorptive compared to the IWO used in TCO selective with buried doping solar cells. Comparing the TCO selective solar cell with the Dopants free solar cell, we note a slight Jscmax enhancement of 0.03 mA/cm^2 , which is attributed to the absence of the 2-nm ultra-thin MoO_x at the front side of the device.

For this work, we assume high-quality c-Si wafers with minimal bulk SRH recombination [1]. Therefore, recombination losses of the c-Si bulk are primarily driven by intrinsic recombination [9,143]. As such, we anticipate a rise in intrinsic recombination with higher doping levels and/or thicker c-Si bulk [8,9,143]. Note that as the volume of the absorber decreases, the total (volumetric) recombination also decreases. Such an effect becomes apparent in Voc calculations. Regarding the Voc contour plots, we note that, for all FBC structures, Voc strongly depends on the c-Si thickness while exhibiting minimal variations with respect to half-pitch values. In general, FBC solar cells with 50-µm thick c-Si bulk exhibit the highest Voc values. Note our simulation range of c-Si bulk thickness starts from a minimum of 50 µm, thus higher Voc values are expected for even lower c-Si thickness values. In Table 5 we compare the Voc_{max} attained for the five FBC architectures under study. The highest Vocmax values were calculated for Dopants free, TCO selective and Localized contacts solar cells, which are all based on i-a-Si:H surface passivation and do not have any in-diffusion region in the bulk. In contrast, both the PERFECT RJ cell and the TCO selective with buried doping cell, which exhibit thin dopant in-diffusion regions within the bulk, demonstrate slightly lower Voc_{max} values because of Auger-Meitner recombination [144] in the vicinity of the c-Si bulk surfaces.

The carrier collection in FBC solar cells involves a collecting path from the generation position within the c-Si bulk to the front and rear contacts. Differently from the fully metallized rear side, for which we expect only a vertical transport path, the collection path of charge carriers reaching the front contact consists of both vertical and lateral components. The vertical transport is influenced by the c-Si thickness, while the lateral transport is determined by the half-pitch of the various solar cell designs. This effect is evident in FF calculations. Concerning FF contour plots, we observe that half-pitch values impact more on the FF trend than c-Si thickness in the Perfect RJ cell and the TCO selective with buried junctions solar cell. Conversely, in the Dopants free, TCO selective and Localized contacts cells, the FF trend is nearly equally dependent on half-pitch and c-Si thickness. In both cases, lower FF values correspond to higher half-pitch values. In the PERFECT RJ and TCO selective with buried junctions cells, lateral transport is supported by highly conductive doped regions near the interfaces. In these designs, a larger half-pitch corresponds to a larger highly doped region, which causes larger variations in the FF with changes in half-pitch compared to variations in c-Si thickness. Indeed, the FF is more sensitive to half-pitch than c-Si thickness for such solar cell designs. In this regard, as the halfpitch increases, the FF decreases. We calculate FF_{max} values close to 86 % and 85.6 % for PERFECT RJ and TCO-selective with buried junctions solar cells, respectively, when the half-pitch is 200 µm. Alternatively, for FBC architectures without supporting doping in the c-Si bulk, the contribution of lateral transport is comparable to that of vertical transport. Highest FF_{max} values are thus attained with thinner c-Si bulk and reduced half-pitch values, as reported in Table 5. Upon evaluating each FBC architecture individually, it is evident that the supporting doping at the interfaces enhances lateral transport, as seen in PERFECT RJ and TCO selective with buried junctions designs. However, this doping also constrains the achievable FF, resulting in lower values compared to structures without doping due to their reduced intrinsic recombination in agreement with ref. [145].

The performance of the FBC architectures under study is driven by the trade-off among three main mechanisms: light management, intrinsic recombination, and lateral carrier transport, each influenced by the half-pitch and c-Si thickness. These mechanisms individually impact Jsc, Voc, and FF within each structure. The result of such competitive mechanisms is observed in the trend of η contour plots. Overall, we observe that η exhibits a bell-shaped trend, reaching its maximum at specific combinations of half-pitch and c-Si thickness for different solar cell designs (see Table 5). By comparing the individual maximum performances, we find that the Localized contacts solar cell design exhibits the most promising results, with efficiencies approaching 28 %. Interestingly, solar cell designs incorporating highly doped regions within the absorber bulk achieve their η_{max} for thicker c-Si bulk compared to other designs. This effect results from an optimal balance between light management and the increased intrinsic recombination in highly doped regions. Additionally, a half-pitch of 400 µm appears to be (near-) optimal among all studied FBC architectures, representing the best trade-off between light management and lateral transport for effective carrier collection.

4.2. Interdigitated back-contacted structures

In contrast to FBC architecture, solar cells with IBC architecture exhibit better optical potential for the absence of front metallization and thin conductive supporting layers. In this part of our work we assess three promising IBC solar cell designs as reported in Fig. 6: (1) the *IBC poly-Si* cell (see Fig. 6 (f)), employing doped poly-Si CSCs for both ETL and HTL rear fingers; (2) the *IBC Hybrid* cell, featuring poly-Si CSC for rear ETL fingers and SHJ CSC for rear HTL fingers (see Fig. 6 (g)); and (3) the *IBC SHJ* cell, incorporating SHJ CSC for both ETL and HTL rear fingers (see Fig. 6 (h)). In all simulated structures, to ensure a consistent



Fig. 8. Simulated Jsc, Voc, FF and η as a function of half pitch and c-Si thickness for IBC solar cells with poly-Si, hybrid and SHJ CSC.

Summary of the maximum values of the external parameters of the three IBC architectures under study, alongside the related pairs of rear metallization pitch and c-Si bulk thickness. Note such pairs change per each external parameter highlighting how different mechanisms of light management, intrinsic recombination, and lateral carrier transport compete in different solar cell designs. Ultimately, the maximum efficiency accounts for the optimal solution.

	Jsc _{max} [mA/cm ²]	Voc _{max} [mV]	<i>FF</i> _{max} [%]	η _{max} [%]
IBC poly-Si IBC Hybrid IBC SHJ	$\begin{array}{l} \mbox{43.56 (Pitch = any } d_{c.Si} = 220 \ \mbox{\mu m}) \\ \mbox{43.58 (Pitch = any } d_{c.Si} = 220 \ \mbox{\mu m}) \\ \mbox{43.69 (Pitch = any } d_{c.Si} = 220 \ \mbox{\mu m}) \end{array}$	$\begin{array}{l} \mbox{766.5 (Pitch = any } d_{c\cdot Si} = 50 \ \mbox{\mu m}) \\ \mbox{766.6 (Pitch = any } d_{c\cdot Si} = 50 \ \mbox{\mu m}) \\ \mbox{767.0 (Pitch = any } d_{c\cdot Si} = 50 \ \mbox{\mu m}) \end{array}$	$\begin{array}{l} 87.67 \ \% \ (Pitch=400 \ \mu m \ d_{c.Si}=50 \ \mu m) \\ 87.50 \ \% \ (Pitch=400 \ \mu m \ d_{c.Si}=50 \ \mu m) \\ 87.56 \ \% \ (Pitch=400 \ \mu m \ d_{c.Si}=50 \ \mu m) \end{array}$	$\begin{array}{l} 28.29 \ \mbox{(Pitch}=400 \ \mbox{\mu m} \ d_{c.Si}=70 \ \mbox{\mu m}) \\ 28.29 \ \mbox{(Pitch}=400 \ \mbox{\mu m} \ d_{c.Si}=60 \ \mbox{\mu m}) \\ 28.41 \ \mbox{(Pitch}=400 \ \mbox{\mu m} \ d_{c.Si}=50 \ \mbox{\mu m}) \end{array}$



Fig. 9. Evolution of efficiency η as a function of wafer resistivity for promising FBC and IBC structures with half pitch and thickness combination.

comparison, we consider fully metallized ETL and HTL fingers, a 5- μ m wide gap between back contacts, 2 Ω cm bulk resistivity, and 80 % of the pitch covered by the HTL. Here we define the pitch as the distance covering the symmetry element between two consecutive ETL or HTL fingers. Later, in Section 4.3, we shall investigate the effect of different HTL width over pitch (*HTL/pitch* ratio). The simulation domain includes solar cells featuring pitch values ranging from 400 to 2000 μ m and c-Si thicknesses values from 50 to 220 μ m. Again, notwithstanding the challenge in eventually realizing solar cells with the most stringent parameters, we consider realistic our simulation ranges.

Fig. 8 presents the contour plots of *Jsc*, *Voc*, *FF*, and η as function of

half-pitch and c-Si thickness for the three IBC solar cell designs under study. For comparative purposes among IBC structures, the results are illustrated on a uniform scale. Overall, we observe consistent trends in the simulated external parameters among all IBC structures.

Looking at the *Jsc*, we observe its values are largely independent from half-pitch variations but are significantly influenced by the c-Si thickness. This behaviour is ascribed to the light management, where the absence of front shadowing renders *Jsc* insensitive to changes in halfpitch values, while c-Si thickness remains the dominant factor. The results indicate that increasing the c-Si thickness leads to higher *Jsc* values. In Table 6, we report the *Jsc*_{max} of the three IBC solar cell designs.

Summary of the maximum efficiency values attainable by the eight solar cell designs under study for bulk resistivity value of 10 Ω cm, alongside the related values of metallization pitch, wafer thickness, wafer resistivity and HTL/pitch ratio (only for IBC designs).

	η_{\max} [%]	Pitch [µm]	d _{c-Si} [μm]	HTL/pitch [%]
PERFECT RJ	27.17 %	800	160	n.a.
Dopants free	27.40 %	800	70	n.a.
TCO selective	27.22 %	600	70	n.a.
TCO selective with buried junctions	26.47 %	800	190	n.a.
Localized contacts	28.00 %	800	60	n.a.
IBC poly-Si	28.53 %	400	70	90 %
IBC Hybrid	28.54 %	400	60	90 %
IBC SHJ	28.64 %	400	50	70 %

Notably, those featuring poly-Si CSC (IBC poly-Si and IBC Hybrid) exhibit slightly lower *Jsc* by 0.1 mA/cm² compared to the IBC SHJ solar cell, due to the rear side light management which includes poly-Si layers that are more absorptive in the infrared region than thin-film silicon layers.

Regarding the Voc, we observe a trend similar to that of FBC solar cells (see Section 4.1). Indeed, Voc decreases significantly with increasing c-Si thickness due to the rise in intrinsic recombination while remaining unaffected by half-pitch variations. In Table 6 we report the Voc_{max} of the three IBC solar cell designs. While such values are close among them, the IBC SHJ cell shows a slightly higher Voc by 0.5 mV, ascribed to the reduced intrinsic recombination in the absence of the highly doped regions characteristic of poly-Si CSC (see Section 2.1). For low values of both half-pitch and c-Si thickness we observe high FF values. We attribute this result to the similar contributions of lateral and vertical components to carrier transport. Given the high-performance nature of the three IBC solar cell designs under study, the found FF_{max} values are very close to each other (see Table 6). Finally, looking at η values, we observe that efficiency increases as both half-pitch and c-Si thickness decrease. Within our simulation domain, the η_{max} is calculated for 200-µm wide half-pitch in all three IBC designs and for bulk thickness between 50 and 70 µm (see Table 6). All simulated IBC solar cell designs exhibit the capability to surpass the 28 % performance threshold.

4.3. Towards the efficiency limit

After analysing the impact of metallization pitch and c-Si thickness



Fig. 11. Efficiency η as a function of HTL/pitch ratio for the three IBC designs under study, considering optimal c-Si thickness (d_{c-Si}) of 70, 60 and 50 μm for IBC poly-Si, IBC Hybrid and IBC SHJ, respectively.

on the performance of FBC and IBC solar cell designs, we further assess the impact of wafer resistivity on their performance. To that end, we selected for each design the pair of pitch and bulk thickness values that maximizes η . Fig. 9 illustrates the efficiency evolution of the eight solar cell designs under study as function of (n-type) wafer resistivities ranging from 1 to 10 Ω cm and different pitch values around to or smaller than the value realizing η_{max} (see previous sections). It is worth noting we choose such resistivity range and pitch values as technologically available in nowadays high-quality c-Si wafers production. Furthermore, in this work, we assume a constant 40 ms SRH lifetime (Table 2) and apply the intrinsic recombination model from Ref. [143]. While the SRH lifetime remains unchanged, intrinsic recombination increases with higher doping concentrations (lower resistivity), reducing the intrinsic lifetime. Consequently, in these simulations, higher-resistivity wafers lead to longer intrinsic and effective lifetimes.

In general, η shows an increase with higher wafer resistivity. This effect is expected because intrinsic recombination is dominant and lower resistivity correlates with higher intrinsic recombination [8,9]. Nevertheless, the improvement in conversion efficiency becomes less



Fig. 10. Power loss analysis and light management assessment for optimal solar cell structures.(a) Contribution of intrinsic and SRH recombination mechanisms to power losses across all optimal designs reported in Table 7. (b) Optical losses evaluation in terms of c-Si absorbed light, shading by metal contacts, reflected light, light parasitically absorbed by front (front par.) and rear (rear par.) supporting layers.



Fig. 12. Efficiency ranking for FBC and IBC designs based on n-type c-Si wafers. Here P stands for pitch (two times half-pitch), d_{bulk} for c-Si thickness, ρ_{bulk} for the wafer resistivity, W_{finger} for the front metallization width, %HTL for the HTL/pitch ratio in IBC designs.

pronounced for resistivity values exceeding 5 Ω cm. For FBC designs, we observe that further narrowing down the pitch to below 600 um does not yield any efficiency increase and, instead, proves to be even detrimental in the pursuit of ultimate practical efficiency. This is linked to a higher light shading at the front side caused by larger metallization fraction. In contrast, for IBC designs, deploying narrower pitches at the rear side not only positively impacts the light management with a wider cumulative reflective area at the back of the device but also enhances lateral charge collection. In Table 7, we report the η_{max} attainable by the eight solar cell designs under study for bulk resistivity value of 10 Ω cm, alongside the related values of metallization pitch, wafer thickness, wafer resistivity and HTL/pitch ratio (only for IBC designs). Furthermore, we calculate the conversion power and light management breakdown, as reported in Fig. 10. We confirm that, for all optimal solar cell structures reported in Table 7, intrinsic recombination mechanisms dominate power losses, as illustrated in Fig. 10a. Regarding optical losses, we observe in Fig. 10b that optimal light management does not necessarily lead to the optimal solar cell. Instead, achieving the best performance requires a proper balance between optical and electrical losses for each solar cell design, considering the material and CSC configuration discussed in Section 2, as well as the subsequent optical optimization.

Finally, in case of IBC designs, while considering fixed the bulk thickness to the optimized values, the bulk resistivity to 10Ω cm and the pitch to 400μ m, we investigate the impact of the HTL/pitch ratio on η in the range from 0.2 to 0.9 (see Fig. 11). Our results reveal that η reaches optimal values of 28.53 % and 28.54 % for a coverage ratio of 0.9 in IBC poly-Si and IBC Hybrid solar cells, respectively. For the IBC SHJ solar cell, the maximum η of 28.64 % is achieved with a HTL/pitch ratio of 70 %. This effect is ascribed to the different trade-offs between lateral transport and recombination mechanisms inherent to each IBC design, as discussed in Refs. [22,64]. In general, the lateral transport of minority carriers (holes) improves with higher HTL/pitch ratio (= more emitter fingers collectively present at the rear side of the device). However, the transport of majority carriers is also affected by higher HTL/pitch ratio, enhancing the recombination of carriers before achieving the n-contact.

Comparing FBC and IBC designs, FBC solar cells exhibit lower η values due to the front metal contact which hinders maximal light incoupling. Among the proposed FBC designs, we note that only the Localized contacts design can achieve 28 % efficiency for a solar cell with a 400 µm half pitch, 60-µm thick c-Si bulk, and 10 Ω cm wafer resistivity. Note that this combination of pitch and c-Si thickness maximizing η stems from the trade-off between lateral transport and

light management, impacting both *FF* and *Jsc*, as shown in Fig. 7. It is worth noting that the inherent performance limitation caused by the front metallized contact can be mitigated by reducing the width of the front contact. In this work, we implement a 10-µm wide front metal contact; but we anticipate further enhancements in FBC performance as developments in the solar cell fabrication process allow for narrower front contacts and more precise patterning. By mitigating the front contact shadowing effect, we predict an optimal c-Si thickness near to 100 µm, with η coming close to the intrinsic limit of 29.6 % or the 29.4 % value consistent with ref. [8,9].

The limitation of front contact shadowing in FBC solar cells is absent for IBC solar cells. Therefore, all simulated IBC designs demonstrate performance well exceeding 28 %. Remarkably, the IBC SHJ solar cell exhibits the highest calculated efficiency in this work. We note that η reaches its maximum for the minimal 400-µm wide pitch, which we have assumed as the lowest value in this study based on current technologically feasible patterning limits. However, pushing further the pitch value to 40 µm, we calculate an efficiency of 28.75 %. Furthermore, in the absence of SRH recombination and optical losses as well as for a 50-µm thick bulk with a resistivity of 1000 Ω cm, we compute with our modelling framework an efficiency of 29.14 %, which is close to the physically predicted c-Si intrinsic limit.

We thus anticipate that further improvements towards the intrinsic efficiency limit of c-Si solar cells can be achieved as developments in the solar cell fabrication process enable narrower patterning features in general and smaller pitches specifically for the IBC architecture. Interestingly, after overcoming patterning limitations, we expect that a 50- μ m thick c-Si bulk will lead to the efficiency limit. Note that the optimal thickness of 100 μ m for c-Si bulk in the FBC architecture is calculated as the optimal trade-off between transport in the wafer and light trapping, given the distance between both contacts, as reported in Ref. [8]. Since in the IBC architecture both contacts are the same side of the device, the optimal 100- μ m long carrier transport path is effectively halved, enabling the use of thinner wafers. This results in lower intrinsic recombination, that is higher *Voc* and *FF*, but potentially lower *Jsc* than their FBC counterparts with similar intrinsic limiting performance.

5. Conclusions

We have systematically elucidated the three key factors behind the concept of carrier-selective contacts (CSC): the work function of the deposited layers, the energy barriers at heterointerfaces, and the energy alignment between energy states through the transport stack. These factors can be rigorously assessed by solving the Poisson equation, offering deep insights into CSC behaviour.

Building on this foundation, we evaluated different CSC designs used in state-of-the-art c-Si solar cells, including poly-Si, SHJ, and dopants free CSCs. We also introduced innovative CSC structures such as the TCO selective CSC and the TCO-selective with buried junctions CSC, providing a detailed understanding of their charge collection mechanisms. We identified the material properties that drive charge transport across these CSCs offering guidelines for future experimental optimization. We thus defined the optimal parameters for CSC and applied them in both FBC and IBC solar cells.

Our study analyzed novel FBC and IBC designs focused on design parameters: metallization pitch, c-Si thickness, and wafer resistivity, assuming reduced Shockley-Read-Hall recombination in high-quality wafers. The simulation results are visually summarized in Fig. 12, where we rank all eight studied solar cell designs. For FBC designs, the natural technological evolution of the TOPCon solar cell, that is the PERFECT RJ design, and the natural evolution of the SHJ solar cells, that is the Localized contacts design, top at 27.17 % and 28 %, respectively. Besides those two designs, the TCO selective and the Dopants free solar cell designs also project efficiency well above 27 % while being potentially cheaper than the previous ones in terms of production (i.e. no high thermal budget processes, limited utilization of plasma-enhanced chemical vapor deposition, and high throughput by removing SHJ doped layers). For IBC designs, with a 400- μ m wide pitch and 10 Ω cm wafer resistivity, we calculated maximum efficiencies of 28.53 %, 28.54 %, and 28.64 % in case of IBC poly-Si, IBC Hybrid and IBC SHJ solar cells, respectively. Our simulation results demonstrate that FBC Localized contacts solar cell and all IBC designs are able to achieve efficiencies equal or higher than 28 %.

Our calculations indicate that patterning limitations are the main technological barrier to achieve the intrinsic efficiency limits in FBC and IBC cells. However, with progress in fabrication technology enabling narrower patterning, we anticipate significant performance enhancement, bringing c-Si solar cells closer to their theoretical efficiency limits. These findings cover not only the current state-of-the-art but also propose a basis for the next generation of high-efficiency c-Si solar cells, anticipating future innovations in photovoltaic technology.

CRediT authorship contribution statement

Paul Procel-Moya: Writing – original draft, Methodology, Conceptualization. **Yifeng Zhao:** Writing – review & editing, Methodology, Conceptualization. **Olindo Isabella:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization.

Data availability statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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