Solar Energy Advances 5 (2025) 100077

Contents lists available at ScienceDirect

Solar Energy Advances

journal homepage: www.elsevier.com/locate/seja

An overview of solar cell simulation tools

Abu Kowsar [a,1,*], Sumon Chandra Debnath [a,1,*], Md. Shafayet-Ul-Islam [a,b], Mohammad Jobayer Hossain [c], Mainul Hossain [b], AFM Kamal Chowdhury [d], Galib Hashmi [e], Syed Farid Uddin Farhad [a]

[a] Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhaka 1205, Bangladesh
[b] Department of Electrical and Electronic Engineering, University of Dhaka, Ramna, Dhaka 1000, Bangladesh
[c] Khulna University of Engineering & Technology (KUET), Khulna 9203, Bangladesh
[d] International University of Business Agriculture and Technology (IUBAT), Uttara, Dhaka 1230, Bangladesh
[e] Institute of Energy, University of Dhaka, Dhaka 1000, Bangladesh

ARTICLE INFO

Keywords:
Solar cell
Device modelling
Simulator
Photovoltaic
Optimization

ABSTRACT

Solar cell simulation software offers an intuitive platform enabling researchers to efficiently model, simulate, analyze, and optimize photovoltaic devices and accelerate desired innovations in solar cell technologies. This paper systematically reviews the numerical techniques and algorithms behind major solar cell simulators reported in the literature. The status, scopes, and limitations of these simulators have been critically evaluated after recording their use in nearly two hundred published articles. For the first time, we present a comparative study of the simulators in terms of their availability, applications, and system requirements. We anticipate that this review will aid in selecting the most appropriate solar cell simulator for the numerical study of preferred type of solar cells.

1. Introduction

Solar energy is one of the most promising clean energy sources and is believed to be an effective alternative to fossil fuels. To harness ubiquitous solar energy effectively, the photovoltaic community has come across different kinds of solar cells; among them, crystalline silicon (c-Si), amorphous silicon (a-Si:H), cadmium telluride (CdTe), copper indium gallium selenide (CIGS), and multijunction solar cells are already in a mature technology stage, and the rest of the cells, such as copper zinc tin sulfide (CZTS), dye-sensitized, perovskite, quantum-dot, copper manganese tin sulfide (CMTS) solar cells, etc., are still in the rudimentary stage [1,2]. Although solar cells have been fabricated using numerous techniques, computer-aided modelling tools or simulators are becoming popular for providing computational assistance to researchers and manufacturers of solar cell growth before actual mass production. Solar cell simulators started their journey in the mid-1980s [3,4]. Rover et al. invented the first popular solar cell simulator, PC1D, for IBM-compatible personal computers in 1985 [4,5]. This simulation tool was designed to visualize the characteristic response of the c-Si solar cells. Although the initial objective for introducing these computer models was to demonstrate the device performance metrics in academia, it has also gradually spread as an essential simulation tool for industrial applications. A list of open-source and commercial packages has been developed explicitly for modelling and numerically simulating solar cells [6]. The PV community currently utilizes numerous one-dimensional (1D) modelling programs, such as AMPS-1D, PC1D, and SCAPS-1D, as well as 2D, 3D modelling tools, such as ASPIN3, COMSOL Multiphysics, DESSIS, Silvaco ATLAS, and ASA [7–9].

Alongside these simulators, clean energy researchers are accustomed to the energy system (comprising single source or hybrid sources) simulation tools, such as PVsyst, HOMER, RETScreen, TRANSYS, etc. [10]. In PV literature, only a handful of review articles have been found on simulators that can optimize and design the energy system, simulate the energy system's performance, and investigate the enviro-techno-economic feasibilities, sensitivity, uncertainty, and risk factors of the energy system [11]. Sinha and Chandel published a review article in 2014 [12] where the authors systematically reviewed 19 hybrid renewable energy system simulators and offered their fundamental insights along with the availabilities and limitations so that PV researchers and practitioners can effectively choose the most suitable simulator for their concerning energy system. Sharma et al. reported

* Corresponding author.
E-mail addresses: apukowsar@gmail.com (A. Kowsar), sumondebnath.bcsir@gmail.com (S.C. Debnath).
[1] Co-first authors contributed equally.

https://doi.org/10.1016/j.seja.2024.100077
Received 15 August 2024; Received in revised form 15 October 2024; Accepted 10 November 2024
Available online 10 November 2024

Nomenclature

ADEPT	A Device Emulation Program and Tool
AFORS-HET	Automat FOR Simulation of HEterostructures
AMPS	Analysis of Microelectronic and Photonic Structure
a-Si:H	Hydrogenated Amorphous Silicon
ASA	Advanced Semiconductor Analysis
ARC	Anti-reflecting Coating
ATLAS	Advanced Technology for Lateral Analysis and Simulation
c-Si	Crystalline Silicon
CdS	Cadmium Sulfide
CdTe	Cadmium Telluride
CIGS	Copper Indium Gallium Selenide
CMTS	Copper Manganese Tin Sulfide
CZTS	Copper Zinc Tin Sulfide
COMSOL	Computer Solution
DSSC	Dye-Sensitized Solar Cell
EQE	External Quantum Efficiency
FDTD	Finite-difference Time Domain
FF	Fill-Factor
HIT	Heterojunction with Intrinsic Thin layer
μc-Si:H	Hydrogenated Microcrystalline Silicon
J_{sc}	Short-circuit Current Density
MJSC	Multijunction Solar Cell
MSCS-1D	One Dimensional Multijunction Solar Cell Simulator
OLED	Organic Light-emitting Diode
OghmaNano	Organic and hybrid Material Nano Simulation tool
PCE	Photoconversion Efficiency
PC1D	Personal Computer One Dimensional
PECSIM	PhotoElectroChemical SIMulation software
PSC	Perovskite Solar Cell
PVsyst	Photovoltaic systems
QDSSC	Quantum Dots Sensitize Solar Cell
QE	Quantum Efficiency
R&D	Research and Development
SCAPS	Solar Cell Capacitance Simulator
SETFOS	Semiconducting Thin Film Optics Simulator
SRH	Shockley-Read-Hall
V_{oc}	Open Circuit Voltage
TCAD	Technology Computer-Aided Design
TCO	Transparent Conducting Oxide
TFSC	Thin-film Solar Cell

another work on the simulation software [10] that reviewed and investigated the simulators that are mainly utilized for solar photovoltaic energy. On the other hand, Milosavljevic et al. reviewed and validated the simulator based on a case study dedicated to and developed for PV energy [13].

However, similar to the review of energy system simulation programs, there is no such work on solar cell simulators so that anyone can effectively select the most appropriate tool for their solar cell fabrication. This article aims to critically review the solar cell simulation tools and delineate the overview of the current status, essential insight, features, scopes, and limitations for identifying the most appropriate simulator for simulating a specific type of solar cell. To the best of the author's knowledge, this is the first comprehensive review of solar cell device simulators. The remaining part of the article is organized as follows: Section 2 presents the simulation procedure used in commercial solar cell simulators and discusses device physics. Section 3 reviews the traditional and newly emerged solar cell simulators, their operating principles, features and limitations. Section 4 presents a comparative analysis of the simulations that help new users choose the right ones for their needs. Section 5 provides the overall conclusions of the study.

2. Solar cell simulation method

The photovoltaic market and literature are enriched with a variety of solar cells, including first-generation Si, second-generation a-Si:H-, CdTe-, CIGS-, CZTS-, CMTS-, CFTS-, DSSC TFSC and advanced perovskite (PSC), tandem, multijunction, quantum dot solar cell etc. [14–16]. These cells are comprised of different layers, including substrate, hole

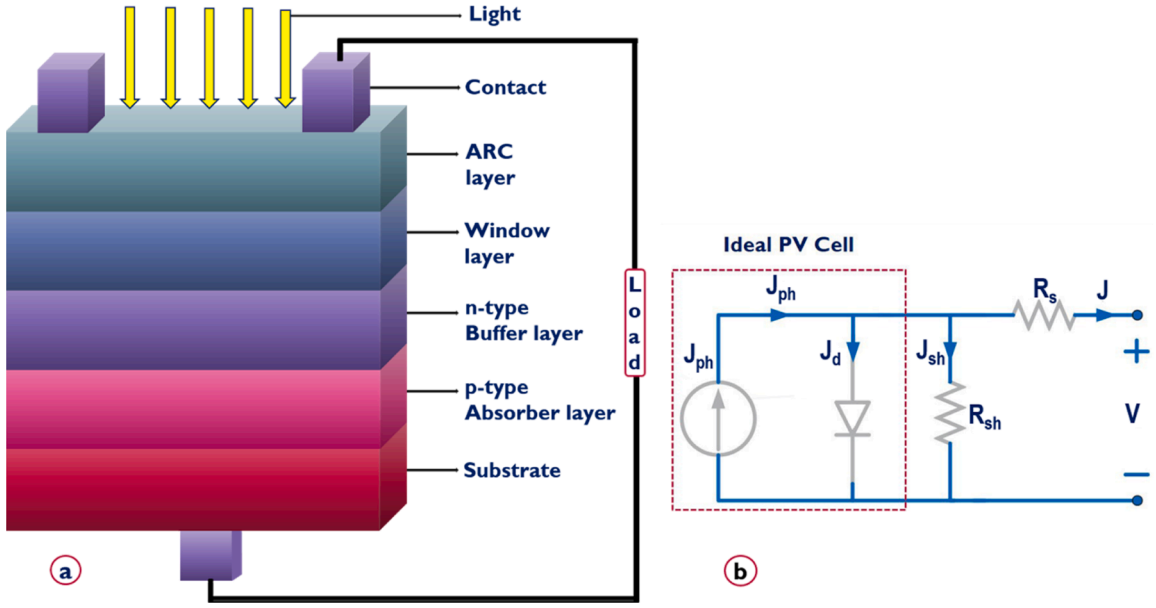

Fig. 1. (a) A typical solar cell device architecture consists of the substrate, p-type absorber, n-type buffer, window, anti-reflecting, and contact layer; (b) Equivalent circuit diagram of this solar cell adopted from Hossain et al. [19].

transport, absorber, buffer, window, electron transport, anti-reflecting coating, and contact layer. A typical solar cell device structure is shown in Fig. 1. First, part of the incident light penetrates the cell and gets absorbed by the active material (i.e., absorber layer), which converts the visible light into electricity. The front side ARC layer reduces reflection from the front surface of the cell. The solar spectrum is broad, ranging from ultraviolet to infrared domain. However, not all the photons are absorbed equally by the absorber layer; only the photons having energy greater than the bandgap energy of the active material are absorbed and can contribute to the electron-hole pair generation. Some of the photogenerated electrons and holes are lost through recombination (in the bulk and the unpassivated surfaces) and resistive losses [17]. Only the remaining electrons and holes are collected by the contacts and can serve as a source of electricity. In Fig. 1(b), J_{ph} represents the photogenerated current density of the cell. Now, part of the electricity generated by the cell will be lost due to the recombination and parasitic absorption losses (expressed by the dark saturation current density, J_d) and the resistive losses (expressed by the series resistance, R_s and the shunt resistance, R_{sh}) [18]. An ideal solar simulator has to consider all these effects: carrier generation rate, optical loss, recombination loss, parasitic absorption loss and resistive loss.

To explain how a solar cell simulator works, let us take the example of the SCAPS-1D modelling software. It was used in the simulation of the potential solar power under ambient conditions [20], considering the normal global solar irradiance AM1.5G with an input power of 1000 W/m^2 and a temperature of 300 K [21,22]. It is possible to utilize a combination of seven different layers as inputs with this tool, and each layer has its own front and back contacts. It facilitates the examination of various device properties, including current-voltage (J–V) characteristics, capacitance-frequency (C–f) and capacitance-voltage (C–V) characteristics, photoconversion efficiency (PCE), open-circuit voltage (V_{oc}), fill-factor (FF), short-circuit-current density (J_{sc}), and quantum efficiency (QE) [23]. The simulator solves Poisson's equation, continuity Eqs. (2) and (3), and drift-diffusion Eqs. (4) and (5) for charge carriers.

$$\frac{dE}{dx} = \frac{p}{\varepsilon} = \frac{q}{\varepsilon}(p(x) - n(x) - N_A + N_D) \tag{1}$$

The basic relationship between electric field strength and charge carrier is established by Eq. (1), where E stands for electric field, ρ for charge density, and ε for material permittivity. In semiconductor technology, the charge is divided into four distinguished constituents, namely, donor concentration (N_D), acceptor concentration (N_A), electron concentration (n), and hole concentration (p).

$$\frac{dn}{dt} = \frac{1}{q}\frac{dJn}{dx} - (U - G) \tag{2}$$

$$\frac{dp}{dt} = -\frac{1}{q}\frac{dJp}{dx} - (U - G) \tag{3}$$

Where U and G denote the recombination and generation rates respectively. Hole and electron current densities are denoted by J_n and J_p.

$$Jn = \mu n n\frac{d\varphi}{dx} + Dn\frac{dn}{dx} \tag{4}$$

$$Jp = \mu p p\frac{d\varphi}{dx} + Dp\frac{dp}{dx} \tag{5}$$

As illustrated in Fig. 2, the simulation procedure starts with selecting an appropriate simulator for any specific solar cell. Therefore, the required optoelectronic properties, including bandgap (E_g), electron affinity (χ), dielectric constant (ε), carrier density (N_c, N_v), carrier mobility (μ_n, μ_p), doping levels (N_A, N_D), and trap densities (N_t), and simulation conditions, including airmass (AM), series (R_s) and shunt resistance (R_{sh}), etc. must be arranged and inserted with the designated dialog boxes.

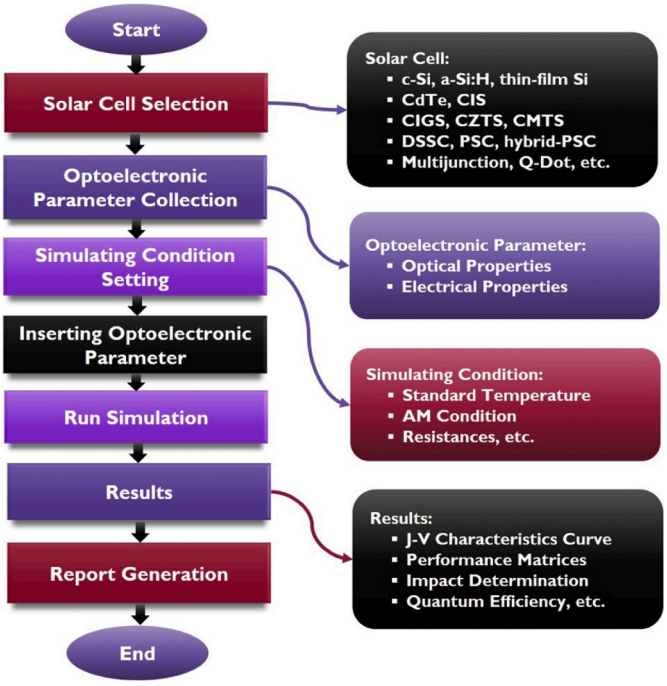

Fig. 2. Schematic illustration: Basic steps for the numerical simulation procedure of a typical solar cell.

The simulator generates a list of results, including band diagram, J-V characteristics curve, V_{oc}, J_{sc}, FF, PCE, and QE, as shown in Fig. 3. Besides the performance metrics, the simulation software can evaluate the impacts of different parameters, such as thickness, absorption, carrier distributions, recombination, etc.

More than fifty such modelling tools have been utilized in academia and industry [10,24]; the present contribution critically reviewed widely used solar cell simulation tools. These simulators solve the standard solar cell equations and models with appropriate boundary conditions, but each tool has some advantages and disadvantages; after knowing the pros and cons of these tools, the readers and researchers can select a simulation tool over the others. The following section sequentially reviews ADEPT, AMPS-1D, AFORS-HET, ASA, ASPIN, OghmaNano, PC1D, PECSIM, SCAPS-1D, SETFOS, Silvaco ATLAS and TCAD, and COMSOL Multiphysics simulators considering the highlights, scopes, limitations, special features, and availability.

3. Review of the solar cell simulators

3.1. ADEPT simulator

The nanoHUB solar cell modelling tool ADEPT is a heavily used computer program written to simulate multiple solar cells, including a-Si:H, CIGS, CZTS, CdTe, etc. [25]. Utilizing a generalized Newton method, this tool discretizes the standard solar cell models on a mesh, linearizes them, determines the unknowns, and performs 1D simulation efficiently. The latest version of the simulator, ADEPT 2.1, advances in sparse matrix solvers that enable 2D simulations to run on a comparatively small workstation and can simulate the homo- and hetero-structures, both abrupt and graded solar cells, such as c-Si, GaAs, AlGaAs/GaAs tandem, and thin film solar cells [26].

The ADEPT simulator includes a detailed model of solar cell physics, including the effects of carrier transport, recombination, and light absorption [27–29]. This allows the tool to accurately predict the functional output of devices and optimize their characteristic under variable conditions [30,31] and materials, such as silicon, III-V compounds, and chalcogenides [32]. It can also be used to model the effects of

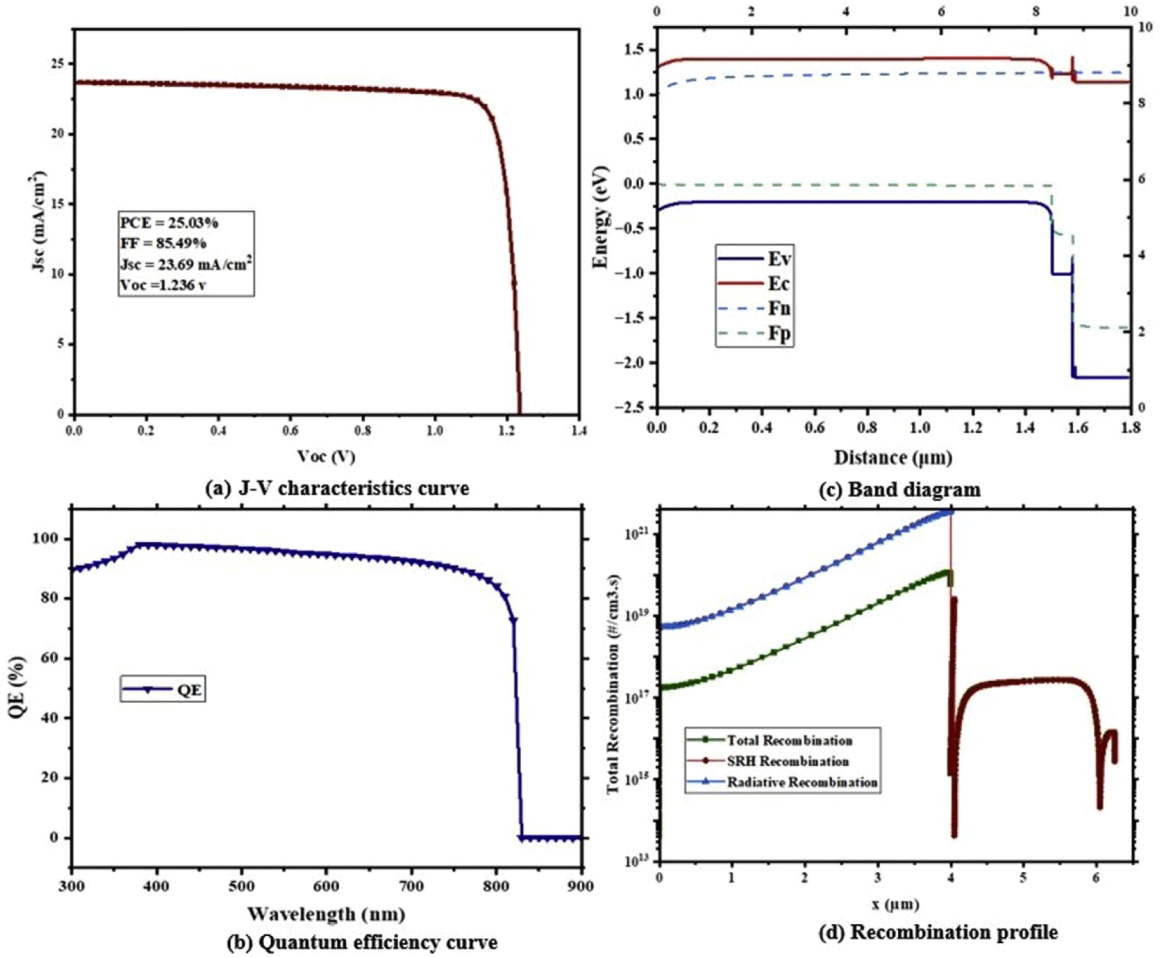

Fig. 3. Simulated results generated from SCAPS-1D, where presents the illuminated (a) J-V characteristic curve, (b) EQE versus wavelength, (c) Energy band levels diagram, and (d) recombination profiles of a solar cell.

temperature and bias voltage on solar cell performance [33]. This freely available tool can be used to calculate a variety of solar cell performance metrics, including PCE, V_{oc}, J_{sc}, and FF [34]]; besides, the effect of bandgap and doping concertation can be investigated [35]. ADEPT offers a comprehensive suite of capabilities to model the effects of defects and impurities in solar cells. It provides a framework for simulating solar cell performance under non-uniform illumination [36]. The simulator does not include interface modelling, band-to-band tunnelling, or modelling of front and back contacts. Additionally, batch processing is not supported, defect and recombination modelling needs to be optimized, some default parameters cannot be changed, and the simulator needs to be more user-friendly than other solar cell simulators.

3.2. *AMPS-1D simulator*

AMPS-1D is also a popular programming software for modelling, designing, and simulating the performance of solar cells, including thin-film poly-silicon pc-Si [37], a-Si:H [38], CIGS [39] and CZTS solar cells [7]. This 1D simulator was developed for two-terminal detectors and single-, poly- and amorphous solar cells analysis using the Newton–Raphson method that enriched it with comparatively superior features than its predecessors. AMPS-1D has been widely utilized for solar cell design, studying the sensitivity of semiconductor parameters, modelling the optimum device structure and determining voltage biasing conditions [40]. At the same time, this tool has been utilized to elucidate the red kink and the transient effect in CdS/CIGS solar cells, modelling thin-film pc-Si cells with reasonable light trapping. Besides, this user-congenial tool can simulate more than one device at a time, where each device is comprised of up to 30 layers with several opto-electronic parameters [41].

The prime data-input parameters of the tool are standard AM1.5 spectra, electron affinity, permittivity, mobility, effective densities, and doping concentration of electrons and holes. Having large numbers and layers, the input parameters entry in AMPS is still tiresome and relatively time-consuming. Moreover, results obtained from the tool are saved on an external file; the inability to save the graphs in popular formats such as PNG and JPEG made the tool more inconvenient. In some cases, increasing the bias voltage can make the model unstable, leading to a complete loss of results [42]. Furthermore, AMPS cannot add a contact layer and substrate or observe its optoelectronic impact on solar cells. To allow fast inputting of optoelectronic data and enhance the visualization of the simulating results aesthetically pleasing, Liu et al. released an updated module of the AMPS simulation software wxAMPS [42]. This updated version can accept identical input data as the originally written AMPS-1D and provides similar physical properties of defects and recombination. In addition, incorporating a trap-assisted tunnelling model makes this software more precise for multijunction solar cell (MJSC) device simulation and optimization. To date, the advanced module, wxAMPS is frequently utilized for simulating and optimizing the CIGS [43], CZTS [44], DSSC [45], CZTS/CTS tandem [46], p–i–n^+/p^+–i–n a-Si:H tandem solar cell [42], and PSC [47] solar cell.

3.3. AFORS-HET simulator

AFORS-HET is an open-source 1D simulator employed to study multilayer homo- or hetero-junction photovoltaics and other optoelectronic devices numerically [48,49]. It was developed in 2003 by A. Froitzheim and his coworkers at Helmholtz-Zentrum Berlin (HZB) in Germany.

This simulator is frequently utilized for modelling and simulating an arbitrary sequence of optoelectronic device layers and interfaces by selecting a number of boundary conditions. This tool also allows multi-dimensional input parameter fitting to synchronize the simulated measurements to actual results. This modelling tool resolves the 1D standard Poisson and transport equations for charge carriers using the finite difference method under a list of geographical conditions for obtaining the optimized solar cell operational performance [50]. Therefore, the prime applications of the simulator are found to evaluate the maximum achievable PCE for the tandem solar cell a-Si:H/c-Si, obtaining design criteria for them and developing measurement methods for examining the a-Si:H/c-Si interface recombination [51,52]. It offers an opportunity to evaluate the function of different optoelectronic parameters present in the fabrication procedure of HIT solar cells [53]. The most recent version of this simulator, named AFORS-HET 2.5, incorporates Auger recombination, Hurkx model, intra-band and Schottky barrier tunnelling through spikes in the conduction and valence bands at interfaces to increase its simulation scope [49].

The application of the AFORS-HET tool is limited to low to medium-doped optoelectronic devices. However, the tool cannot accurately model and simulate the highly doped poly-silicon materials and transparent conductive oxide (TCO) layers [49]. Moreover, the various contact resistance measuring techniques like TLM (transfer length method) or Cox measurements cannot be dealt with by AFORS-HET [54]. In addition, this simulator does not take into account some of the crucial characteristics related to intermediate buffer layers in multilayer cell structures [55].

3.4. ASA simulator

The ASA is an exceptionally designed solar cell simulator package for modelling multilayer amorphous and crystalline semiconductor devices [56]. This 1D steady-state device simulator, written in the ANSI C, was developed by Zeman et al. [57] at the Delft University of Technology. An integrated optoelectrical approach has been incorporated into the software. The optical model, termed 'GenPro (GP)', computes photo-generated charge carriers' generation profiles in devices with smooth and/or uneven surfaces [58]. The optical model comes in four different versions in this tool for modelling smooth and rough semiconductor interfaces, analyzing ray and wave optics combination effect, and incoherent and semi-coherent treatment.

The electrical model of the ASA simulator solves the semiconductor equations to provide insight into the transport system. The defect-pool model allows the user to calculate the defect-states distribution in the solar cell, making ASA an ideal optimization tool for thin-film, c-Si wafer-based and tandem solar cells. The current version of this simulator, ASA7 [59], is available with a web-based user interface and can be used for performing the fast simulation of the JV curves, fill factors and efficiencies of thin-film a-Si:H [60] and μc-Si:H solar cells [61].

3.5. ASPIN simulator

ASPIN is a comprehensive numerical simulator used to simulate transport at heterojunction semiconductor devices under steady-state conditions. The development process of this simulation program started in the late 80′s of the past century [62] at the University of Ljubljana [63]. The conventional drift-diffusion model (Poisson's continuity and charge transport linearized differential equations) and the thermionic-field emission model make up the foundation of this tool. Hence, a multi-layer heterostructure's internal electrical characteristics and other external properties can be computed accurately [64]. The modified Gummel algorithm has been incorporated into the simulator to decrease execution time while maintaining identical precision levels and increasing robustness. Moreover, inserting the trap-assisted tunnelling theory into this simulator facilitates the treatment of a p-i-n/p-i-n tandem cell as a whole.

The current iteration of the software is ASPIN3, which enables 2D analysis of structures. It permits the simulation of lateral transport, grain boundaries, and mixing of various materials [65]. ASPIN3 boosts its modelling strength by considering Auger, SRH, and dangling bond recombination mechanisms. Moreover, ohmic and Schottky contacts and isolating surfaces are the contact interfaces it supports. ASPIN3, in integration with the SunShine optical simulator, has been intensively used to simulate a-Si:H/μc-Si:H and CIGS solar cells [66,67]. The 2D geometry of ASPIN3 is limited to the rectangular structure only [65]. Moreover, this tool cannot be used to simulate a textured TCO layer since a particular optical model would be required for it [68].

3.6. OghamNano simulator

OghamNano is a cross-platform optoelectronic solar cell simulator that can be utilized to simulate the performance metrics of PSCs, polymer-, c-Si-, a-Si:H- and CIGS solar cells [69]. OghmaNano was formerly known as Gpvdm, developed by the C++ platform, supported by Python, and freely accessible to users. To achieve precise and accurate modelling, OghamNano employs advanced techniques, including drift-diffusion and transfer matrix models for organic solar cells [70]. The simulation of perovskite solar cells incorporates mobile ion models and is enhanced through ray tracing models [71,72]. Moreover, it offers automatic fitting to experimental data, facilitating the extraction of crucial parameters for accurate model calibration [73,74]. Its capabilities extend to various optoelectronic measurements, both transient and steady-state, such as dark/light JV curves, CELIV transients, dark/light photo-CELIV transients, transient photocurrent and voltage, intensity-modulated photocurrent spectroscopy, and voltage transients of arbitrary shapes [75,76]. Furthermore, OghamNano encompasses EQE calculation, Suns-V_{oc}, Suns-J_{sc}, and PL/EL measurements, allowing for a comprehensive assessment of device performance under different conditions [77,78]. The platform empowers researchers and engineers to observe the effect of numerous optoelectronic properties on device performance, including mobility, energetic disorder, doping, and recombination [79,80].

OghamNano boasts an array of powerful physical models, a highly optimized multi-trap level SRH solver, and effective circuit models for arbitrary circuits [81,82]. Band-to-band recombination is considered, and the platform supports ray tracing, transfer matrix models, voltage transients of arbitrary shapes, and calculation of reflection profiles [83]. A 3D thermal solver and interface dipole doping model also contribute to the platform's robust simulation capabilities [84,85]. The solver might require enhanced convergence because of the complex mathematical solutions involved in drift diffusion. If the solver is given a problem that is hard to solve, it may need help finding the answer accurately, resulting in errors. The solver may show an error if the electron/hole trap state and carrier concentrations are set below the default value.

3.7. PC1D simulator

The widely utilized simulation software, PC1D, is specifically designed to optimize the first-generation c-Si solar cells [86]. This is the first solar cell simulation tool written in the Pascal language and installed on IBM-compatible personal computers [3,4]. However, currently, it allows users to simulate the electrical and optical behaviour of various types of solar cells, including homo-junctions, hetero--junctions, and tandem cells [87–90]. The simulation speed, user

interface and continual updates to the latest cell models are responsible for its wide use [91]. To develop the primitive version of the PC1D simulator, the Newton-Gummel method, as well as the intra-band and trap-assisted tunnelling model, was employed. Nevertheless, the latest version (imd-PC1D 6.0) of this simulator employs Fermi-Dirac statistics [92] and a number of some of the latest models, such as light absorption, carrier diffusion, drift, and recombination models for performing solar cell efficiency modelling, simulation, optimization, characterization, and impact investigation [93,94].

PC1D provides tools for characterizing and modelling material properties such as the energy bandgap, refractive index, and doping concentration. It allows users to extract important parameters of solar cells, such as the ideality factor, series resistance, and shunt resistance, from experimental data. PC1D calculates and predicts the performance parameters of solar cells, including the I-V characteristics, V_{oc}, J_{sc}, FF, PCE, etc. [95]. The software facilitates the optimization of solar cell parameters to maximize device performance. For example, a c-Si solar cell with 20.35% PCE has been simulated using a PC1D simulator [96]. It enables users to study the effect of various design and process parameters on cell performance, such as the effect of bandgap and electron affinity of ZnO on the overall performance of n-ZnO/p-Si solar cells [97], the impact of ARC layers on c-Si- and CdTe- solar cell [87,98], emitter- and base-thickness, and doping density [95] etc. have been investigated.

The PC1D tool has been utilized for numerous computational applications for first- and second-generation solar cells. The software assists in predicting the performance of different solar cell configurations, allowing researchers to compare and evaluate various designs before fabrication [99]. This software aids in studying the impact of material properties and composition on solar cell performance, enabling researchers to explore new materials to improve device efficiency. Besides these numerous scopes, the user experiences few limitations during the simulation using this tool. PC1D utilizes simplified models to simulate solar cell behaviour, which may only capture some of the complexities and nuances present in real-world devices. This tool is primarily a 1D simulation software, assuming the modelled devices are homogeneous along the vertical axis. Additionally, there is no option to observe the effect of bus bars and fingers on the solar cells, which carry the current from the individual solar cells.

3.8. PECSIM simulator

Dr Matthias Schmid and his research team at Zürich University of Applied Sciences developed the state-of-the-art PECSIM simulator for solar cells, especially analyzing and optimizing dye-synthesized solar cells (DSSCs) [100]. The simulator can only be used with a valid license for either Mathematica or Mathematica Player Pro. A comprehensive electrical and optical model that describes all physiochemical and optical processes of DSSC serves as the foundation for PECSIM. The ray-tracing algorithm [101] based optical model considers the successive internal light reflections within the cell and the antireflection coating characteristics. The injection, transportation, and recombination of charge carriers are taken into account in the electrical model. The simulator offers four parameter-driven modules: steady-state, impedance, transient, and loss analysis. The cell's time-dependent characteristics and output power, the transient decay of photocurrent and photovoltage, and the standard measurement of losses due to optical and electrical processes can be accurately modelled by these modules.

PECSIM facilitates the user in computing some solar cell performance parameters, like J-V curve, Jsc, Voc, FF, PCE, and quantum efficiency. The quantitative study of energy conversion losses provided by the tool helps to improve the stability and overall efficiency of the DSSC. Moreover, the software can be used to implement the coupled optical and electrical model of the quantum dots-sensitized solar cells [102]. A congenial graphical user interface is provided by PECSIM so that a user can quickly understand the complex interactions among the different components of the solar cell. Hence, it facilitates the development of solar cell optimization strategies.

3.9. SCAPS-1D simulator

SCAPS-1D is another frequently used tool specially developed for second-generation solar cells, including CIGS- and CdTe-based solar cells [103]. The application of this program has been extended to c-Si cells, thin-film GaAs-, a-Si:H- and micromorphous Si solar cells [104]. Developers have provided a dedicated website and repository where users can access the latest versions of SCAPS 1D. This open-source program is freely available [22].

The key features of SCAPS include accommodating up to 7 semiconductor layers and the option to grade almost all parameters based on local composition or cell depth. It includes parameters like electron affinity (χ), dielectric constant (ε), bandgap (E_g), carrier distributions (N_c, N_v), threshold voltages (V_{thn}, V_{thp}), carrier mobility (μ_n, μ_p), doping (N_A, N_D), and trap densities (N_t) [22]. Besides, it incorporates graded band gaps and a new model for intra-band tunnelling, improving the accuracy of current transport simulations. SCAPS considers various recombination mechanisms and defect levels in materials and interfaces, accounting for their charge state and impact on recombination [22,104]. It also takes into account the optical properties of defect levels, enabling the study of impurity photovoltaic effects and metastable transitions between defects [105]. Tunnelling effects are considered, including intra-band tunnelling and tunnelling to and from interface states [106]. The tool now simulates multivalent defects, addressing limitations of other tools, and provides accurate modelling of their effect on solar cell performance [107–111]. It can also model meta-stabilities in thin film solar cells based on chalcopyrite materials, accurately simulating the behaviour of intrinsic defects undergoing configuration changes and lattice relaxations [112–114]. Carriers can be generated internally or through user-defined inputs, and various illumination sources are available [115]. SCAPS calculates energy bands, carrier concentrations, and currents at specific working points, enabling analysis of J-V characteristics, AC impedance, and spectral response [16]. The tool also allows for easy calculation of admittance spectra and facilitates the interpretation of admittance data by comparing them with capacitance-voltage measurements [116,117]. SCAPS supports batch calculations, offers customization options, and provides an intuitive user interface with additional features like curve fitting and interpreting admittance measurements [118,119]. The ultra-high PCE and other CZTS solar performances have been simulated using SCAPS-1D [120].

The program does not account for interference phenomena or optical confinement, such as texture and ray tracing. Despite its strengths, the program struggles to achieve convergence at high forward voltages. Additionally, SCAPS is limited to performing calculations in the frequency domain and cannot calculate transient phenomena. Handling interference phenomena, optical confinement effects, and texture using ray tracing would enable more realistic simulations involving light-matter interactions. Enhancing convergence at high forward voltages would ensure stability and reliable results under extreme operating conditions. Introducing time domain calculations would allow the analysis of transient phenomena, providing a comprehensive understanding of device behaviour.

3.10. SETFOS simulator

The solar cell simulator package, SETFOS, can be employed to model the electrical and optical properties of semiconductor devices. This powerful and CPU-efficient simulator written in Java [121] was developed by Professor Ruhstaller, Fluxim AG [122], and specifically designed to create cutting-edge thin-film optoelectronic technologies. The latest version of this commercial software, SETFOS 5.4, was released in July 2023.

The simulator has been developed mainly to study organic semiconductor-based solar cells [123], perovskites [124] and other thin

film devices [125]. The emission, drift-diffusion, absorption, and advanced optics modules are incorporated here to simulate various optical properties and charge transport characteristics. Using multi-target and multi-variable optimization allows the user to look inside devices in ways that cannot be done through experiments. This helps the user understand device performance. In order to simulate the scattering, absorption, and re-emission of light from nanoparticles or a quantum dot film, this tool also offers a 2D ray-tracing engine [126]. A hardware platform for the universal characterization of various solar cells and OLEDs, called Paios [122], can be combined with SETFOS to introduce an integrated simulation-characterization approach in AC, DC, and transient domains and also for parameter extraction and model validation. This software's speed, reliability, and flexibility facilitate a variety of solar cell applications, particularly in optimizing device structures or in the fundamental research of device physics.

3.11. Silvaco ATLAS and TCAD

ATLAS is a flexible and expandable platform designed for simulating 1D, 2D, and 3D semiconductor devices. The framework is built using contemporary software engineering methods, emphasizing reliability, maintainability, and extensibility. Several mathematical models and equations, including Poisson's equation, carrier continuity equations, and transport equations, along with a discretization of the equations, are implemented in ATLAS such that they can be employed with the finite element grid that serves as the simulation domain's representation. The equations are efficiently solved by the general-purpose device simulator, providing precise and dependable semiconductor device simulation results [127]. The tool is developed by a combination of C and C++ and is used in conjunction with VWF interactive and automation tools, along with ATHENA, UTMOST and SMARTSPACE. All forms of Single junction, multifunction silicon, thin film, perovskite, organic, quantum dot and III-V compound solar cells can be simulated by Silvaco ATLAS.

This ATLAS simulator offers a comprehensive range of features, including DC, AC small-signal, and full-time-dependent simulations [128]. It encompasses drift-diffusion and dynamic transport models, considering lattice heating [129,130]. Heterojunctions with graded and abrupt bandgaps, amorphous and polycrystalline materials, and optoelectronic interactions with ray tracing are supported by the simulator [131,132]. It accommodates general circuit environments, considers stimulated emission and radiation, and incorporates Fermi-Dirac and Boltzmann statistics [133,134]. Advanced mobility models, heavy doping effects, and full acceptor and donor trap dynamics are included [135,136].

The simulator handles various contact types (Ohmic, Schottky, insulating), considers SRH, radiative, Auger, and surface recombination, and impacts ionization effects [137,138]. It accounts for floating gates, band-to-band and Fowler-Nordheim tunnelling, hot carrier injection, and quantum transport models [139–141]. Thermionic emission currents are also modelled in the simulation [142,143]. Users specify problems, defining the structure, models, and bias conditions for simulation. Defects, trap, and recombination models are usable only for thin-film with thin-film transistor products. ATLAS can predict electrical characteristics based on physical structures and bias conditions. It is quicker, cost-effective, and offers information not easily measurable.

TCAD is a well-established and trusted solution for thousands of users from diverse fields in the semiconductor industry [144]. The optical module of the simulator is a specialized 2D and 3D tool that focuses on modelling light absorption and photoelectric effects in nonplanar semiconductor devices. TCAD can simulate monocrystalline and polycrystalline silicon solar cells with thin-film and tandem models. The program is developed by a C++ platform along with the Silvaco parameter library. Users can access the software with an annual subscription, academic and evaluation license.

Silvaco TCAD software can be used to study the impact of changing the thicknesses of the p-type and n-type contact regions in Si-solar cells [145]. This tool assists the users in exploring the performance characteristics of thin film solar cells that consist of a-SiC:H, μc-Si, and a-SiGe:H layers [146]. Besides, Silvaco TCAD is utilized to investigate the effects of 3-D texturing in Si-solar cells, aiming to enhance optical absorption [147]. This tool has also been utilized to investigate the impact of surface texturing on GaAs-solar cells to address the optical losses that have been limiting the overall efficiency of photovoltaic devices [148]. In addition, TCAD is used to study and analyze the performance limits of tandem micromorph (a-Si:H/μc-Si:H) and triple-junction (a-Si:H/a-SiGe:H/μc-Si:H), polymer, perovskite solar cells [149–153] and investigate and optimize of ultrathin CIGS solar cells [154].

Simulation and performance optimization of n-type Interdigitated back contact Silicon heterojunction (IBC-SiHJ) solar cells can also be studied using this software, along with quantum dot solar cells [133,155]. Simulation of partial dopant-free asymmetric silicon heterostructure solar cells (P-DASH) can be conducted by Silvaco TCAD [156]. This tool can also be utilized to investigate the influence of base doping level, size and grain-boundary effect, double back surface field layer consequences, electrical characteristics of Passivated Emitter and Rear Contact (PERC) solar cell, recombination effects, the impact of phosphorus ion implantation, the effect of the heavily doped silicon wafer, light trapping mechanism, effect of microscopic defect, the effect of protonic radiation [157–166].

TCAD is computationally expensive, especially for 3D simulations with complex geometries. Users must have a good understanding of semiconductor physics, device modelling, and simulation techniques to use this tool effectively. The accuracy of the simulations depends on the accuracy of the device models, which are typically based on experimental data. Therefore, users need to have a good understanding of the underlying physical processes and accurate material parameters to achieve reliable and meaningful results.

3.12. COMSOL multiphysics

COMSOL Multiphysics simulation package has been rarely used in simulating solar cell structures until recently [167]. Unlike 1-D simulation platforms like SCAPS or AMPS, COMSOL can perform thermal analysis and heat distribution mapping to the surrounding environment and other conducting layers. The semiconductor module in COMSOL allows it to solve the drift-diffusion model of carrier transportation. The electromagnetic waves module maps the optical photogeneration profile, while the heat-transfer module maps and analyses the thermal profile across the device structure. These modules can be coupled together to simultaneously produce a combined output containing photogeneration, recombination and heat profile in three dimensions (3D). Integrating optical-electrical-thermal modules provides a comprehensive understanding of the underlying device physics involved. Modelling complex structures in 3D and combining all three modules can offer significant challenges in terms of computational resources and the user's expertise level.

4. Comparative analysis

For performing successful simulation, most of the simulator receives the input dataset, including solar irradiance, layer thickness, dielectric constant, bandgap, electron affinity, electron and hole mobility, the density of states, carrier distribution, defect density, etc. [168,169]. It generates performance metrics, such as short-circuit current, reverse saturation current, current-voltage characteristics response, open circuit voltage, maximum power point, fill factor, and efficiency. More than 50 such simulators have been found in the literature, but it takes much work to choose an appropriate one [24,170,171]. These solar cell simulators employ different sets of semiconductor equations or models to solve the required performance metrics of several kinds of solar cells. This article elucidates the overall simulation procedure of SCAPS-1D with proper illustrations for Cu_2MnSnS_4 (CMTS) solar cells in section

2. However, an attempt has been made to critically review the research methods that are used in the simulation tools, especially for the visualization of the impacts of using different simulators on the achievable results from similar initial data sets or common scenarios that could strengthen the arguments for recommendations for which type of simulator is more suitable for which type of solar cells. But, considering the volume of the review work, it is impractical to describe all results from 12 simulators individually in a single report with practical examples. Therefore, the present review summarizes the scope, availability, and limitations to facilitate the selection of the most appropriate simulation tool for the numerical study of solar cells. The study has revealed that PC1D is the baseline programming tool for the c-Si solar cell. One-dimensional AMPS is an easy-to-access tool, mainly utilized for thin-film devices, but its data input procedure is comparatively time-consuming. To resolve this issue, an advanced program of AMPS-1D, wxAMPS, offers the user a congenial data entry interface. This tool offers advanced capabilities for modelling materials with high defect densities, band tails, and other characteristics commonly observed in thin film photovoltaics compared to the SCAPS-1D [42].

Nevertheless, the SCAPS-1D simulator can consider the defect parameters of the 1st and 2nd generation solar cells; this unique feature made the tool more reliable in producing relatively accurate performance metrics than the others. Besides these frequently used tools, the ASA simulator is the best for amorphous devices, and OghmaNano, PECSIM, and SETFOS have been employed mostly for organic solar cells, and AFROS-HET, ATLAS, and TCAD are frequently utilized for heterojunction solar cells. Among the genres, ADEPT, AMPS-1D, SCAPS-1D, and TCAD simulators have the capability to perform simulations for multiple solar cell devices. Besides the single-junction solar cell simulations, ADEPT, ASA, SETFOS, ATLAS, and TCAD tools possess additional features to simulate comparatively lower-efficiency tandem cells. However, advanced TCAD and wxAMPS simulation software versions have additional features to simulate III-V multijunction solar cells. However, these tools have been developed based on the standard model of the single-junction solar cells; recently, a new simulation tool, MSCS-1D, has been released for high-efficiency multijunction solar cells [172] that has been developed using the dedicated multi-junction solar cell model. Table 1 compares the different simulators with respect to the inventor, availability, development platform, system requirements and available features.

Besides these well-established 12 simulators, recently, the PV community has also been utilizing other tools, including DFT [187], FDTD investigation [188], and MATLAB [189] for the simulation of different solar cells. In addition, a list of new simulation tools has been introduced recently, such as CoBoGUI, EDNA, Lumerical, Microwave Studio, Optiwave, PC3S, Quokka, QS Cell, MSCS-1D, OPV lab, SARAH (IBC), Solcore, Solis, etc. Table 2 briefly describes the recently released comparatively less-known solar cell simulation software.

5. Conclusion

The present contribution provides an overview of the leading solar cell simulation programs, detailing their scope, availability, and limitations. Notably, advancements in computer capacity and speed have significantly enhanced the features, speed, applications, and availability of these simulators in recent years. The overall simulation procedure has been explained with an example simulator model being used for an emerging solar cell, which gives a clear idea of how these simulators work and calculate device parameters. Additionally, it includes a comparative analysis of the simulators to identify the most suitable simulation tools for extracting characteristic parameters. This systematic review is expected to assist the photovoltaic community in selecting the appropriate simulator tool for numerically exploring novel cell structures, and their fabrications for accelerated development. Furthermore, this study is expected to serve as a valuable reference for modelling, simulation, characterization, and in-depth analysis of the

Table 1
Comparative summary of the solar cell simulators.

Simulator	Inventor	Availability	Development Platform	System Requirements	Simulating features
ADEPT	Gray *et al.* [25, 173]	Free of cost	FORTRAN 77	Windows, MAC, Linux	c-Si SC, FTSC including, CIGS, OVC/CIGS, CdTe, a-Si:H, GaAs, and AlGaAs/GaAs tandem SC
AMPS-1D	Fonash *et al.* [40,174]	Free of cost	FORTRAN	Windows 95/98/2000/NT and XP, recent versions	c-Si, TFSC including, a-Si:H, CIGS, CZTS, and PSCs. Additionally, it can simulate and analyze the different impacts that affect solar cell
AFORS-HET	Froitzheim *et al.* [48,175]	Free of cost	FORTRAN, C	Linux, Windows NT, 95 and more recent versions	a-Si:H, n-$MoSe_2$/p-Si and a-Si:H/c-Si tandem SCs
ASA	Zeman *et al.* [176,177]	Paid	FORTRAN (Old version), C (New version)	Windows 95/98/Me, NT3.5/ NT4/2000/ Vista/7 or Linux	a-Si:H, In addition: μc-Si:H, PSC/Si and a-Si:H/μc-Si:H tandem SC
ASPIN	Smole *et al.* [178,179]	Free of cost	C, Python	Linux, macOS, and FreeBSD	a-Si:H In addition: CIGS, a-Si:H/C-Si. a-Si:H p-i-n heterojunction solar cell
Ogham Nano	MacKenzie et al [180]	Free of cost	C++, Python	Windows	Polymer, C-Si, a-Si:H, PSC, and CIGS solar cells.
PC1D	Rover *et al.* [4, 181]	Free of cost	FORTRAN, C	Windows 95/98/ME/XP/NT	1st gen c-Si SC, but having capability to simulate most of the SC, including tandem ($In_{0.2}Ga_{0.8}N$/p-Si) SC. It can simulate and analyze the different impacts on solar cell.
PECSIM	Schmid *et al.* [100,182]	Free of cost	Mathematica	Windows, MAC	DSSC, Quantum Dots Sensitize Solar Cells (QDSSCs), and PSC
SCAPS-1D	Burgelman *et al.* [20,183]	Free of cost	C++	Windows 95, 98, NT, 2000, XP, Vista, Windows 7 and recent versions	2nd gen TFSC, including, CIGS-, CdTe-, a-Si:H, $Cu_2FeSnSe_4$, $Cu_2MnSnSe_4$, GaAs-, μc-Si- SC, and tandem cell
SETFOS	Ruhstaller [122, 184]	Paid	Java	Windows, MAC	Organic solar cell; Additionally, PSC, QDs, PSC/Si tandem SCs
Silvaco ATLAS	Ivan Pesic [185, 186]	Paid	C, C++	Window, MAC	Organic solar cell, CZTS, tandem solar cell, photodetector
TCAD	Ivan Pesic [150, 185]	Paid	C, C++, FORTRAN	Windows, Linux, MacOS	CMOS, power, memory, image sensors, solar cells, and analog/RF devices

Table 2
Brief description of newly developed solar cell simulators.

Simulator	Inventor and Organization	Features
CoBoGUI	Eidlloth *et al.,* [190] ISFH	This tool is a script collection based on MATLAB and COMSOL that can simulate c-Si-, concentrator-, and thin-film solar cell but not feasible to simulate organic and perovskite solar cell.
EDNA	McIntosh *et al.,* [191] Australian National University	This tool analyses the recombination and collection associated with phosphorus or boron emitter, can determine the emitter saturation current and the collection current of an emitter diffusion with Fermi Dirac statistics but models work only for crystalline silicon solar cell.
PC3S	Paul A. Basore [192] PV Specialist Services	PC3S was developed on MS Excel to calculate surface parameters, specific to silicon crystalline solar cells, such as 3D surface texture, doping profiles, surface recombination velocity, and optical surface coatings, which serve as inputs for PC3D.
Quokka	Andreas Fell [193] Australian National University	This simulation tool was developed on MATLAB to simplify charge carrier transport equations, result in a model that is computationally inexpensive without a loss of generality for silicon solar cell only.
QS Cell	Cuevas *et al.*, [194] Australian National University	This tool was developed for modelling characterization of silicon wafer and solar cells in the context of the impact of carries mobility and recombination on device performance.
MSCS-1D	Kowsar *et al.*, [172] BCSIR	This tool is developed for multijunction solar cell, is capable to modelling and simulation of III-V based tandem, and MJSC, but cannot simulate the performance matrix of single junction solar cell.
OPV lab	Ray *et al.*, [195] Purdue University, NNC	The tool simulates the I-V characteristics of organic solar cells with bilayer or planar heterojunction configuration with flux at D-A interface carrier generation and bi-molecular recombination, but does not have any defect model.
SARAH (IBC)	Saint-Cast *et al.*, [196] Fraunhofer ISE	SARAH employs the diffusion resistance concept and the superposition principle to simulate the prevalent IBC cell design, featuring line p+ and n+ diffusions and a front surface field.
Solcore	Alvarez *et al.,* [197] Imperial College of London	This tool provides a multi-scale, Python-based library for modelling solar cells (III-V, Si, Ge, Sn) and semiconductor alloy materials but cannot calculate multi junction characteristics under radiative coupling and illumination condition.
Solis	Sidi Hamady [198] Université de Lorraine	This tool implements drift-diffusion transport model, various recombination's, supports anode and cathode parameters, and handles spontaneous and piezoelectric polarization, allowing flexibility in simulating heterostructure solar cells but cannot simulate tandem cell.

influence of different parameters on the performance metrics of solar cells.

CRediT authorship contribution statement

Abu Kowsar: Writing – original draft, Visualization, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Sumon Chandra Debnath:** Writing – original draft, Visualization, Data curation, Conceptualization. **Md. Shafayet-Ul-Islam:** Writing – original draft, Resources, Data curation. **Mohammad Jobayer Hossain:** Writing – review & editing, Visualization, Validation, Formal analysis. **Mainul Hossain:** Writing – review & editing, Validation, Supervision, Formal analysis. **AFM Kamal Chowdhury:** Writing – review & editing, Validation, Formal analysis. **Galib Hashmi:** Writing – original draft, Validation, Resources. **Syed Farid Uddin Farhad:** Writing – review & editing, Supervision, Formal analysis.

Declaration of competing interest

The authors hereby affirm the absence of any conflicts of interest and assert that they hold no affiliations or associations with the software products under examination in this paper. The research has been conducted with an unwavering commitment to scientific integrity, with no intent to advocate or critique any particular software solution.

Acknowledgements

This material is based upon the regular R&D work financially supported by the BCSIR under grant number 39.02.0000.011.14.169.2023/IERD-10.

Data availability

Associated data can be provided on reasonable request.

References

[1] M. Fazal, S. Rubaiee, Progress of PV cell technology: feasibility of building materials, cost, performance, and stability, Solar Energy 258 (2023) 203–219.
[2] J. Ramanujam, et al., Flexible CIGS, CdTe and a-Si: H based thin film solar cells: a review, Prog. Mater. Sci. 110 (2020) 100619.
[3] P.A. Basore, D. Rover, A. Smith, PC-1D version 2: Enhanced numerical solar cell modelling, in: Conference Record of the Twentieth IEEE Photovoltaic Specialists Conference, IEEE, 1988, pp. 389–396.
[4] D. Rover, P. Basore, G. Thorson, Solar cell modeling on personal computers, IEEE Photovol. Specialists Confer. 18 (1985) 703–709.
[5] P.A. Basore, D.A. Clugston, PC1D version 4 for Windows: from analysis to design, in: Conference Record of the Twenty Fifth IEEE Photovoltaic Specialists Conference-1996, IEEE, 1996, pp. 377–381.
[6] Y. Liu, M. Ahmadpour, J. Adam, J. Kjelstrup-Hansen, H.-G. Rubahn, M. Madsen, Modeling multijunction solar cells by nonlocal tunneling and subcell analysis, IEEe J. Photovolt. 8 (5) (2018) 1363–1369.
[7] A. Haddout, A. Raidou, M. Fahoume, A review on the numerical modeling of CdS/CZTS-based solar cells, Appl. Phys. A 125 (2019) 1–16.
[8] G.L.M. Tcheum, A.T. Ngoupo, S. Ouédraogo, N. Guirdjebaye, J.M.B. Ndjaka, Numerical analysis of ultrathin Cu (In, Ga) Se 2 solar cells with Zn (O, S) buffer layer, Pramana 94 (1) (2020) 111.
[9] D. Parajuli, G.S. Gaudel, KC Debendra, K.B. Khattri, W.Y. Rho, Simulation study of TiO2 single layer anti-reflection coating for GaAs solar cell, AIP. Adv. 13 (8) (2023).
[10] W. Ma, X. Xue, and G. J. E. Liu, "Techno-economic evaluation for hybrid renewable energy system: application and merits," vol. 159, pp. 385-409, 2018.
[11] M. Lalwani, D. Kothari, M. Singh, Investigation of solar photovoltaic simulation softwares, Int. J. Appl. Eng. Res. 1 (3) (2010) 585–601.
[12] S. Sinha, S. Chandel, Review of software tools for hybrid renewable energy systems, Renew. Sustain. Energy Reviews 32 (2014) 192–205.
[13] D.D. Milosavljević, T.S. Kevkić, S.J. Jovanović, Review and validation of photovoltaic solar simulation tools/software based on case study, Open Physics 20 (1) (2022) 431–451.
[14] A. Kowsar et al., "Progress in major thin-film solar cells: Growth technologies, layer materials and efficiencies," vol. 9, no. 2, pp. 579-597, 2019.
[15] A. Kowsar, S.C. Debnath, M.S. Islam, A.N. Bahar, S.F.U. Farhad, Numerical simulation of the high efficiency triple junction concentrator photovoltaic cells

using MSCS-1D, in: 2021 IEEE 48th Photovoltaic Specialists Conference (PVSC), IEEE, 2021, pp. 0722–0725.
[16] A. Isha, A. Kowsar, et al., High efficiency Cu2MnSnS4 thin film solar cells with SnS BSF and CdS ETL layers: a numerical simulation, Heliyon. 9 (5) (2023).
[17] M.J. Hossain, M. Sun, K.O. Davis, Photon management in silicon photovoltaic cells: a critical review, Solar Energy Mater. Solar Cells 267 (2024) 112715.
[18] M.J. Hossain, et al., A comprehensive methodology to evaluate losses and process variations in silicon solar cell manufacturing, IEEe J. Photovolt. 9 (5) (2019) 1350–1359.
[19] M. J. Hossain, "Measurement and mitigation of optical, recombination and resistive losses in silicon photovoltaics," 2021.
[20] A. Niemegeers, M. Burgelman, Effects of the Au/CdTe back contact on IV and CV characteristics of Au/CdTe/CdS/TCO solar cells, J. Appl. Phys. 81 (6) (1997) 2881–2886.
[21] M. Burgelman et al., "SCAPS manual most recent.pdf".
[22] M. Burgelman, K. Decock, A. Niemegeers, J. Verschraegen, S. Degrave, SCAPS manual, University of Ghent, Ghent, Belgium, 2016.
[23] A. Kowsar, et al., Enhanced photoconversion efficiency of Cu2MnSnS4 solar cells by Sn-/Zn-based oxides and chalcogenides buffer and electron transport layers, Solar Energy 265 (2023) 112096.
[24] P. Lighthouse, Overview of PV simulation programs. PV Lighthouse, 2024. https://www.pvlighthouse.com.au/simulation-programs. accessed October 07.
[25] J.L. Gray, Adept: a general purpose numerical device simulator for modeling solar cells in one-, two-, and three-dimensions, in: The Conference Record of the Twenty-Second IEEE Photovoltaic Specialists Conference-1991, IEEE, 1991, pp. 436–438.
[26] J. Gray, X. Wang, R. V. K. Chavali, X. Sun, A. Kanti, and J. R. Wilcox, "ADEPT 2.1," 2011.
[27] J.E. Moore, C.J. Hages, R. Agrawal, M.S. Lundstrom, J.L. Gray, The importance of band tail recombination on current collection and open-circuit voltage in CZTSSe solar cells, Appl. Phys. Lett. 109 (2) (2016).
[28] A. Ibrahim, Study of Au/n-Tiˆ sub 2ˆ S/p-Si/Al Schottky-type thin film heterojunction solar cells: computer simulation modeling, Am. J. Appl. Sci. 12 (4) (2015) 262.
[29] C.J. Hages, N.J. Carter, R. Agrawal, Generalized quantum efficiency analysis for non-ideal solar cells: Case of Cu2ZnSnSe4, J. Appl. Phys. 119 (1) (2016).
[30] Y. Zhu, A. Perna, P. Bermel, Optimizing Device Characteristics for VLS-Grown InP Heterojunction Solar Cells, in: 2019 IEEE 46th Photovoltaic Specialists Conference (PVSC), IEEE, 2019, pp. 1083–1088.
[31] S. Tobbeche, S. Kalache, M. Elbar, M.N. Kateb, M.R. Serdouk, Improvement of the CIGS solar cell performance: structure based on a ZnS buffer layer, Opt. Quantum. Electron. 51 (2019) 1–13.
[32] R.V.K. Chavali, E.C. Johlin, J.L. Gray, T. Buonassisi, M.A. Alam, A framework for process-to-module modeling of a-Si/c-Si (HIT) heterojunction solar cells to investigate the cell-to-module efficiency gap, IEEe J. Photovolt. 6 (4) (2016) 875–887.
[33] M. Asaduzzaman, A.N. Bahar, M.M.R. Bhuiyan, M.A. Habib, Impacts of temperature on the performance of CdTe based thin-film solar cell, in: IOP conference series: materials science and engineering 225, IOP Publishing, 2017 012274.
[34] M. B. Hosen, M. K. Ali, M. Asaduzzaman, A. Kowsar, and A. N. J. I. J. R. E. R. Bahar, "Performance optimization of ZnS/CIGS solar cell with over 25% efficiency enabled by using a CuIn3Se5 OVC layer," vol. 10, no. 4, pp. 2000-2005, 2020.
[35] M. Asaduzzaman, M. Hasan, A.N. Bahar, An investigation into the effects of band gap and doping concentration on Cu (In, Ga) Se 2 solar cell efficiency, Springerplus. 5 (2016) 1–8.
[36] R.V.K. Chavali, J.V. Li, C. Battaglia, S. De Wolf, J.L. Gray, M.A. Alam, A Generalized Theory Explains the Anomalous Suns–$ V_ {{\rm {oc}}} $ Response of Si Heterojunction Solar Cells, IEEe J. Photovolt. 7 (1) (2016) 169–176.
[37] A. Belfar, R. Mostefaoui, AMPS-1D in a-Si: H/μc-Si: H tandem solar cells, J. Appl. Sci. 11 (16) (2011) 2932.
[38] N. Hernandez-Como, A. Morales-Acevedo, Simulation of hetero-junction silicon solar cells with AMPS-1D, Solar Energy Mater. Solar Cells 94 (1) (2010) 62–67.
[39] A. Bouloufa, K. Djessas, A. Zegadi, Numerical simulation of CuInxGa1− xSe2 solar cells by AMPS-1D, Thin. Solid. Films. 515 (15) (2007) 6285–6287.
[40] H. Zhu, A.K. Kalkan, J. Hou, S.J. Fonash, Applications of AMPS-1D for solar cell simulation, in: AIP Conference Proceedings 462, American Institute of Physics, 1999, pp. 309–314.
[41] I.S. Mokgosi, Solar Cell Device Simulations from Ab Initio Data and the Implementation of Efficiency Enhancing Techniques, University of the Witwatersrand, Faculty of Science, School of Physics, 2019.
[42] Y. Liu, Y. Sun, A. Rockett, A new simulation software of solar cells—wxAMPS, Solar Energy Mater. Solar Cells 98 (2012) 124–128.
[43] S. Yaşar, S. Kahraman, S. Çetinkaya, Ş. Apaydın, İ. Bilican, İ. Uluer, Numerical thickness optimization study of CIGS based solar cells with wxAMPS, Optik. (Stuttg) 127 (20) (2016) 8827–8835.
[44] S. Çetinkaya, Study of electrical effect of transition-metal dichalcogenide-MoS2 layer on the performance characteristic of Cu2ZnSnS4 based solar cells using wxAMPS, Optik. (Stuttg) 181 (2019) 627–638.
[45] J. He, T. Zhang, P. Tang, C. Qiu, X. Feng, X. Luo, Simulation on the carrier transport process inside the semiconductor of dye sensitized solar cells by wxAMPS software, Electrochim. Acta 125 (2014) 218–224.
[46] M.A. Olopade, O.O. Oyebola, A.D. Adewoyin, D.O. Emi-Johnson, Modeling and simulation of CZTS/CTS tandem solar cell using wxAMPS software, in: 2015 IEEE 42nd Photovoltaic Specialist Conference (PVSC), IEEE, 2015, pp. 1–4.
[47] N.A. Sultana, M.O. Islam, Z.H. Mahmood, Utilization of low cost metals as back contact with Perovskite Solar Cell, Dhaka Uni. J. Appl. Sci. Eng. 4 (1) (2017) 35–38.
[48] A. Froitzheim, R. Stangl, L. Elstner, M. Kriegel, W. Fuhs, AFORS-HET: a computer-program for the simulation of heterojunction solar cells to be distributed for public use, in: 3rd World Conference onPhotovoltaic Energy Conversion, 2003. Proceedings of 1, IEEE, 2003, pp. 279–282.
[49] R. Varache, C. Leendertz, M. Gueunier-Farret, J. Haschke, D. Muñoz, L. Korte, Investigation of selective junctions using a newly developed tunnel current model for solar cell applications, Solar Energy Mater. Solar Cells 141 (2015) 14–23.
[50] R. Huang, M. Yu, Q. Yang, L. Zhang, Y. Wu, Q. Cheng, Numerical simulation for optimization of an ultra-thin n-type WS2/p-type c-Si heterojunction solar cells, Comput. Mater. Sci. (2020) 109600.
[51] R. Stangl, M. Kriegel, M. Schmidt, AFORS-HET, Version 2.2, a numerical computer program for simulation of heterojunction solar cells and measurements, in: 2006 IEEE 4th World Conference on Photovoltaic Energy Conference 2, IEEE, 2006, pp. 1350–1353.
[52] W. van Sark, L. Korte, F. Roca, Physics and technology of amorphous-crystalline heterostructure silicon solar cells, Springer, 2012.
[53] N. Dwivedi, S. Kumar, A. Bisht, K. Patel, S. Sudhakar, Simulation approach for optimization of device structure and thickness of HIT solar cells to achieve~ 27% efficiency, Solar energy 88 (2013) 31–41.
[54] Y. Zeng, et al., Theoretical exploration towards high-efficiency tunnel oxide passivated carrier-selective contacts (TOPCon) solar cells, Solar Energy 155 (2017) 654–660.
[55] A. Maslov, V. Mishustin, A. Piryugin, N. Vishnyakov, Physical model to calculate current-voltage characteristics of double-junction solar cells based on a-Si: H and a-SiC: H, in: 2018 7th Mediterranean Conference on Embedded Computing (MECO), IEEE, 2018, pp. 1–4.
[56] M. Burgelman, J. Verschraegen, S. Degrave, P. Nollet, Modeling thin-film PV devices, Progr. Photovol. Res. Applic. 12 (2-3) (2004) 143–153.
[57] M. Zeman, J. Willemen, L. Vosteen, G. Tao, J. Metselaar, Computer modelling of current matching in a-Si: H/a-Si: H tandem solar cells on textured TCO substrates, Solar Energy Mater. Solar Cells 46 (2) (1997) 81–99.
[58] M. Zeman, R. Van Swaaij, J. Metselaar, R. Schropp, Optical modeling of a-Si: H solar cells with rough interfaces: Effect of back contact and interface roughness, J. Appl. Phys. 88 (11) (2000) 6436–6443.
[59] tudelft, ASA Software, Delft University of Technology., 2020. https://www.tudelft.nl/en/eemcs/the-faculty/departments/electrical-sustainable-energy/photovoltaic-materials-and-devices/software-platform/asa-software/(accessed, 27th September.
[60] A. Dagamseh, B. Vet, P. Šutta, M. J. S. E. M. Zeman, and S. Cells, "Modelling and optimization of a-Si: H solar cells with ZnO: Al back reflector," vol. 94, no. 12, pp. 2119-2123, 2010.
[61] B. Pieters, H. Stiebig, M. Zeman, R. Van Swaaij, Determination of the mobility gap of intrinsic μ c-Si: H in p-i-n solar cells, J. Appl. Phys. 105 (4) (2009) 044502.
[62] M. Vukadinovic, J. Krc, K. Brecl, F. Smole, M. Topic, Modelling and simulation of optoelectronic devices with ASPIN, in: The IEEE Region 8 EUROCON 2003. Computer as a Tool 1, IEEE, 2003, pp. 474–477.
[63] F. Smole, M. Topič, J. Furlan, Amorphous silicon solar cell computer model incorporating the effects of TCO/a-Si: C: H junction, Solar Energy Mater. Solar Cells 34 (1-4) (1994) 385–392.
[64] G. Černivec, A. Jagomägi, F. Smole, M. Topič, Numerical and experimental indication of thermally activated tunneling transport in CIS monograin layer solar cells, Solid. State Electron. 52 (1) (2008) 78–85.
[65] "ASPIN3." University of Ljubljana. http://lpvo.fe.uni-lj.si/en/software/aspin3/(accessed 25 August, 2020).
[66] M. Vukadinović, F. Smole, M. Topič, R. Schropp, F.A. Rubinelli, Transport in tunneling recombination junctions: A combined computer simulation study, J. Appl. Phys. 96 (12) (2004) 7289–7299.
[67] J. Krc et al., "Optical and electrical modeling of Cu (In, Ga) Se 2 solar cells," vol. 38, pp. 1115-1123, 2006.
[68] M. Topič, F. Smole, J. Furlan, E. Fortunato, R. Martins, Analysis of front contact heterojunction in a-Si: H one-dimensional position sensitive detectors, Rev. Sci. Instrum. 68 (3) (1997) 1377–1381.
[69] R.C. MacKenzie, T. Kirchartz, G.F. Dibb, J. Nelson, Modeling nongeminate recombination in P3HT: PCBM solar cells, J. Phys. Chem. C 115 (19) (2011) 9806–9813.
[70] A.K. Mishra, R. Shukla, Simulation of photovoltaic material (donor blends PTB7: PC70BM) polymer for solar cell application, Mater. Today: Proc. 46 (2021) 2288–2293.
[71] A. K. Mishra and R. J. M. T. P. Shukla, "Simulation of photovoltaic material (donor blends PTB7: PC70BM) polymer for solar cell application," vol. 46, pp. 2288-2293, 2021.
[72] X. Rodríguez-Martínez, E. Pascual-San-José, M. J. E. Campoy-Quiles, and E. Science, "Accelerating organic solar cell material's discovery: high-throughput screening and big data," vol. 14, no. 6, pp. 3301-3322, 2021.
[73] R. MacKenzie, et al., Loss mechanisms in high efficiency polymer solar cells, Adv. Energy Mater. 6 (4) (2016) 1501742.
[74] F. Deschler, D. Riedel, B. Ecker, E. von Hauff, E. Da Como, R.C. MacKenzie, Increasing organic solar cell efficiency with polymer interlayers, Phys. Chem. Chem. Phys. 15 (3) (2013) 764–769.

[75] Z. Liu, Z. Jin, G. Li, X. Zhao, A. J. E. C. Badiei, and Management, "Study on the performance of a novel photovoltaic/thermal system combining photocatalytic and organic photovoltaic cells," vol. 251, p. 114967, 2022.

[76] R. C. MacKenzie et al., "Interpreting the density of states extracted from organic solar cells using transient photocurrent measurements," vol. 117, no. 24, pp. 12407-12414, 2013.

[77] J. Zhao, et al., Simulation of crystalline silicon photovoltaic cells for wearable applications, IEEe Access. 9 (2021) 20868–20877.

[78] B. Xiao, P. Calado, R.C. MacKenzie, T. Kirchartz, J. Yan, J. Nelson, Relationship between fill factor and light intensity in solar cells based on organic disordered semiconductors: The role of tail states, Phys. Rev. Appl. 14 (2) (2020) 024034.

[79] D. Jalalian, A. Ghadimi, and A. J. J. o. O. N. Kiani Sarkaleh, "Investigation of the effect of band offset and mobility of organic/inorganic HTM layers on the performance of Perovskite solar cells," vol. 5, no. 2, pp. 65-78, 2020.

[80] M. Sittirak, J. Ponrat, K. Thubthong, P. Kumnorkaew, J. Lek-Uthai, Y. Infahsaeng, The effects of layer thickness and charge mobility on performance of FAI: MABr: PbI2: PbBr2 perovskite solar cells: GPVDM simulation approach, J. Phys. Confer. Ser. 1380 (1) (2019) 012146. IOP Publishing.

[81] M. Amir, M.P. Singh, I. Masood, Effect of Exciton dissociation and recombination losses in perovskite photovoltaic cells, in: 2023 International Conference on Power, Instrumentation, Energy and Control (PIECON), IEEE, 2023, pp. 1–6.

[82] D. Puspita, R.D. Syarifah, N.S. Rizal, GPVDM simulation of thickness effect on power conversion efficiency of PEDOT: PSS/P3HT: PCBM solar cell performance, in: AIP Conference Proceedings 2663, AIP Publishing, 2022.

[83] S.G. Daniel, B. Devu, C. Sreekala, Active layer thickness optimization for maximum efficiency in bulk heterojunction solar cell, in: IOP Conference Series: Materials Science and Engineering 1225, IOP Publishing, 2022 012017.

[84] S. Muniandy, M.I.B. Idris, Z.A.F.B.M. Napiah, M. Rashid, The effect of pH level and annealing temperature on NiO thin films as hole transport material in inverted perovskite solar cells, in: 2022 IEEE International Conference on Semiconductor Electronics (ICSE), IEEE, 2022, pp. 13–16.

[85] O. Ourahmoun, Effect of the interfacial materials on the performance of organic photovoltaic cells, Mater. Today: Proc. 49 (2022) 992–996.

[86] P. P. J. J. o. c. e. Altermatt, "Models for numerical device simulations of crystalline silicon solar cells—a review," vol. 10, pp. 314-330, 2011.

[87] D. KC, D. K. Shah, A. M. Alanazi, and M. S. J. J. o. E. M. Akhtar, "Impact of different antireflection layers on cadmium telluride (CdTe) solar cells: a PC1D simulation study," vol. 50, pp. 2199-2205, 2021.

[88] S. Meenakshi, S. Baskar, Design of multi-junction solar cells using PC1D, in: 2013 International Conference on Energy Efficient Technologies for Sustainability, IEEE, 2013, pp. 443–449.

[89] A. Ali, A. Wazira, S. Ahmad, K. Sopian, S.H. Zaidi, PC1D analysis of thin-film crystalline Si x Ge 1− x/Si solar cells, in: 2014 IEEE 40th Photovoltaic Specialist Conference (PVSC), IEEE, 2014, pp. 1317–1320.

[90] H. Haug, B. R. Olaisen, Ø. Nordseth, and E. S. J. E. P. Marstein, "A graphical user interface for multivariable analysis of silicon solar cells using scripted PC1D simulations," vol. 38, pp. 72-79, 2013.

[91] G. S. Thirunavukkarasu et al., "Optimization of mono-crystalline silicon solar cell devices using PC1D simulation," vol. 14, no. 16, p. 4986, 2021.

[92] H. Haug, A. Kimmerle, J. Greulich, A. Wolf, E. S. J. S. e. m. Marstein, and s. cells, "Implementation of fermi–dirac statistics and advanced models in PC1D for precise simulations of silicon solar cells," vol. 131, pp. 30-36, 2014.

[93] H. Haug, J. Greulich, A. Kimmerle, E.S. Marstein, PC1Dmod 6.1–state-of-the-art models in a well-known interface for improved simulation of Si solar cells, Solar Energy Mater. Solar Cells 142 (2015) 47–53.

[94] B. Singh and V. J. M. T. P. Gupta, "Modelling and simulation of silicon solar cells using PC1D," vol. 54, pp. 810-813, 2022.

[95] X. Cai, X. Zhou, Z. Liu, F. Jiang, and Q. J. O. Yu, "An in-depth analysis of the silicon solar cell key parameters' optimal magnitudes using PC1D simulations," vol. 164, pp. 105-113, 2018.

[96] G. Hashmi, A.R. Akand, M. Hoq, H. Rahman, Study of the enhancement of the efficiency of the monocrystalline silicon solar cell by optimizing effective parameters using PC1D simulation, Silicon 10 (4) (2018) 1653–1660.

[97] B. Hussain, A. Aslam, T.M. Khan, M. Creighton, B. Zohuri, Electron affinity and bandgap optimization of zinc oxide for improved performance of ZnO/Si heterojunction solar cell using PC1D simulations, Electronics. (Basel) 8 (2) (2019) 238.

[98] G. Hashmi, M.J. Rashid, Z.H. Mahmood, M. Hoq, M.H. Rahman, Investigation of the impact of different ARC layers using PC1D simulation: application to crystalline silicon solar cells, J. Theor. Appl. Phys. 12 (4) (2018) 327–334.

[99] K. Knutsen, R. Schifano, E. Marstein, B. Svensson, and A. Y. J. p. s. s. Kuznetsov, "Prediction of high efficiency ZnMgO/Si solar cells suppressing carrier recombination by conduction band engineering," vol. 210, no. 3, pp. 585-588, 2013.

[100] S. Wenger, M. Schmid, G. Rothenberger, A. Gentsch, M. Gratzel, J.O. Schumacher, Coupled optical and electronic modeling of dye-sensitized solar cells for steady-state parameter extraction, J. Phys. Chem. C 115 (20) (2011) 10218–10229.

[101] S. Wenger, M. Schmid, G. Rothenberger, M. Grätzel, J. Schumacher, Model-based optical and electrical characterization of dye-sensitized solar cells, in: Proceedings of the 24th European Photovoltaic Solar Energy Conference and Exhibition, CONF, 2009.

[102] M. Hekmat, F. Rostamian, and A. J. M. S. i. S. P. Shafiekhani, "Improving solar cells characteristics by tuning the density distribution of deep trapping states using Au@ DLC decorated on photoanodes," vol. 128, p. 105782, 2021.

[103] M. Burgelman, P. Nollet, S. Degrave, Modelling polycrystalline semiconductor solar cells, Thin. Solid. Films. 361 (2000) 527–532.

[104] M. Burgelman, K. Decock, S. Khelifi, A. Abass, Advanced electrical simulation of thin film solar cells, Thin. Solid. Films. 535 (2013) 296–301.

[105] J. Verschraegen, M. Burgelman, Numerical modeling of intra-band tunneling for heterojunction solar cells in SCAPS, Thin. Solid. Films. 515 (15) (2007) 6276–6279.

[106] M. Burgelman, J. Marlein, Analysis of graded band gap solar cells with SCAPS, in: Proceedings of the 23rd European Photovoltaic Solar Energy Conference, Valencia, Citeseer, 2008, pp. 2151–2155.

[107] M. Kumar, A. Raj, A. Kumar, A. Anshul, Computational analysis of bandgap tuning, admittance and impedance spectroscopy measurements in lead-free MASnI3 perovskite solar cell device, Int. J. Energy Res. 46 (8) (2022) 11456–11469.

[108] A.L. Efros, V.G. Karpov, Electric power and current collection in semiconductor devices with suppressed electron–hole recombination, ACS. Energy Lett. 7 (10) (2022) 3557–3563.

[109] A. Hassan, et al., Recent defect passivation drifts and role of additive engineering in perovskite photovoltaics, Nano Energy (2022) 107579.

[110] F. Arkan, M. Izadyar, Recent theoretical progress in the organic/metal-organic sensitizers as the free dyes, dye/TiO2 and dye/electrolyte systems; Structural modifications and solvent effects on their performance, Renew. Sustain. Energy Rev. 94 (2018) 609–655.

[111] N. Kaur, J. Madan, R. Pandey, Low lead all-inorganic hybrid perovskite: a study of interface defects using SCAPS-1D, in: 2023 IEEE Devices for Integrated Circuit (DevIC), IEEE, 2023, pp. 108–112.

[112] I. Repins, et al., Large metastability in Cu (In, Ga) Se2 devices: The importance of buffer properties, Progr. Photovoltaics: Res. Applic. 27 (9) (2019) 749–759.

[113] K. Decock, S. Khelifi, M. Burgelman, Modelling multivalent defects in thin film solar cells, Thin. Solid. Films. 519 (21) (2011) 7481–7484.

[114] K. Decock, P. Zabierowski, M. Burgelman, Modeling metastabilities in chalcopyrite-based thin film solar cells, J. Appl. Phys. 111 (4) (2012).

[115] A. Niemegeers, M. Burgelman, Numerical modelling of ac-characteristics of CdTe and CIS solar cells, in: Conference Record of the Twenty Fifth IEEE Photovoltaic Specialists Conference-1996, IEEE, 1996, pp. 901–904.

[116] M.S. Lyam, et al., Dominant recombination path in low-bandgap kesterite CZTSe (S) solar cells from red light induced metastability, J. Appl. Phys. 129 (20) (2021).

[117] M.J. Baniyounis, W.F. Mohammed, R.T. Abuhashhash, Analysis of power conversion limitation factors of Cu (In x Ga1−x)(Se) 2 thin-film solar cells using SCAPS, Mater. Renew. Sustain. Energy 11 (3) (2022) 215–223.

[118] M.K. Hossain, et al., An extensive study on multiple ETL and HTL layers to design and simulation of high-performance lead-free CsSnCl3-based perovskite solar cells, Sci. Rep. 13 (1) (2023) 2521.

[119] T. Azizi, H. Toujeni, M.B. Karoui, R. Gharbi, A comprehensive device modeling of solid state dye sensitized solar cell with SCAPS-1D, in: 2019 19th International Conference on Sciences and Techniques of Automatic Control and Computer Engineering (STA), IEEE, 2019, pp. 336–340.

[120] M. A. J. S. E. Rahman, "Enhancing the photovoltaic performance of Cd-free Cu2ZnSnS4 heterojunction solar cells using SnS HTL and TiO2 ETL," vol. 215, pp. 64-76, 2021.

[121] M. T. Neukom, "Charge carrier dynamics of methylammonium lead-iodide perovskite solar cells," *arXiv preprint arXiv:1611.06425,* 2016.

[122] A. Fluxim, "Semiconducting thin film optics simulator SETFOS," Website: http://www.fluxim.com.

[123] S. Bi, Z. Ouyang, S. Shaik, D. Li, Effect of donor-acceptor vertical composition profile on performance of organic bulk heterojunction solar cells, Sci. Rep. 8 (1) (2018) 1–9.

[124] K.-M. Chiang, B.-W. Hsu, Y.-A. Chang, L. Yang, W.-L. Tsai, H.-W. Lin, Vacuum-deposited organometallic halide perovskite light-emitting devices, ACS. Appl. Mater. Interfaces. 9 (46) (2017) 40516–40522.

[125] R. Lampande, G.W. Kim, M.J. Park, B.Y. Kang, J.H. Kwon, Efficient light harvesting in inverted polymer solar cells using polymeric 2D-microstructures, Solar Energy Mater. Solar Cells 151 (2016) 162–168.

[126] B. Blülle, S. Altazin, B. Frouin, L. Stepanova, S. Jenatsch, B. Ruhstaller, 37.4: Light conversion and scattering properties of QD films for display applications: Angle-resolved optical spectroscopy and numerical simulation, in: SID Symposium Digest of Technical Papers 50, Wiley Online Library, 2019, pp. 407–410.

[127] I. Silvaco, ATLAS user's manual, 5, Santa Clara, CA, Ver, 2011.

[128] F. Jahanshah, K. Sopian, Y. Othman, H. Fallah, pn Junction depth impact on short circuit current of solar cell, Solar energy 83 (9) (2009) 1629–1633.

[129] M. Mehrabian, S. Dalir, 11.73% efficient perovskite heterojunction solar cell simulated by SILVACO ATLAS software, Optik. (Stuttg) 139 (2017) 44–47.

[130] A. Hima, N. Lakhdar, B. Benhaoua, A. Saadoune, I. Kemerchou, F. Rogti, An optimized perovskite solar cell designs for high conversion efficiency, Superlattices. Microstruct. 129 (2019) 240–246.

[131] D. Diouf, J. Kleider, T. Desrues, P.-J. Ribeyron, Effects of the front surface field in n-type interdigitated back contact silicon heterojunctions solar cells, Energy Procedia 2 (1) (2010) 59–64.

[132] G. Sahoo, G. Mishra, Design and modeling of an SJ infrared solar cell approaching upper limit of theoretical efficiency, Int. J. Modern Phys. B 32 (02) (2018) 1850014.

[133] M. Belarbi, M. Beghdad, A. Mekemeche, Simulation and optimization of n-type interdigitated back contact silicon heterojunction (IBC-SiHJ) solar cell structure using Silvaco Tcad Atlas, Solar Energy 127 (2016) 206–215.

[134] M.W. Bouabdelli, F. Rogti, M. Maache, A. Rabehi, Performance enhancement of CIGS thin-film solar cell, Optik. (Stuttg) 216 (2020) 164948.

[135] A. Meftah, A. Meftah, N. Sengouga, S. Khelifi, The AlxGa1− xAs window composition effect on the hardness improvement of a p+–n–n+ GaAs solar cell

exposed to the electron irradiation, Energy Convers. Manage 51 (8) (2010) 1676–1678.
[136] G. González-Díaz, et al., Intermediate band mobility in heavily titanium-doped silicon layers, Solar Energy Mater. Solar Cells 93 (9) (2009) 1668–1673.
[137] H. Noge, K. Saito, A. Sato, T. Kaneko, M. Kondo, Two-dimensional simulation of interdigitated back contact silicon heterojunction solar cells having overlapped p/i and n/i a-Si: H layers, Jpn. J. Appl. Phys. 54 (8S1) (2015) 08KD17.
[138] M. Baudrit, C. Algora, Tunnel diode modeling, including nonlocal trap-assisted tunneling: a focus on III–V multijunction solar cell simulation, IEEe Trans. Electron. Devices 57 (10) (2010) 2564–2571.
[139] M. Verma, G.P. Mishra, High electric field sensing in ultrathin SiO_2 and tunnel region to enhance GaInP/Si dual junction solar cell performance, IEEe Sens. J. 22 (2) (2021) 1273–1279.
[140] S. Almosni, et al., Material challenges for solar cells in the twenty-first century: directions in emerging technologies, Sci. Technol. Adv. Mater. 19 (1) (2018) 336–369.
[141] P. Babu, T. Padmanabhan, M. Ahamed, A. Sivaranjani, Studies on copper indium selenide/Zinc sulphide semiconductor quantum dots for solar cell applications, Chalcogenide Letters 18 (11) (2021).
[142] N.E.I. Boukortt, S. Patanè, Y.M. Abdulraheem, Numerical investigation of CIGS thin-film solar cells, Solar Energy 204 (2020) 440–447.
[143] N.E.I. Boukortt, M. Adouane, R. AlHammadi, High-performance ultrathin Cu (In, Ga) Se2 solar cell optimized by silvaco tools, Solar Energy 228 (2021) 282–289.
[144] S. ATLAS, Victory TCAD solution semiconductor process and device simulation, Silvaco Atlas (2023). https://silvaco.com/tcad/#product_briefs. accessed 20 July.
[145] M. Abdullah, N. Rashied, M. Rusop, Layer thickness analysis of silicon solar cells, in: 2010 International Conference on Electronic Devices, Systems and Applications, IEEE, 2010, pp. 149–153.
[146] S. Chang, M. Tang, R. He, W.-C. Wang, Z. Pei, C.-Y. Kung, TCAD simulation of hydrogenated amorphous silicon-carbon/microcrystalline-silicon/hydrogenated amorphous silicon-germanium PIN solar cells, Thin. Solid. Films. 518 (6) (2010) S250–S254.
[147] F. Jahanshah, et al., An investigation of three-dimensional texturing in silicon solar cells for enhanced optical absorption, in: 2008 33rd IEEE Photovoltaic Specialists Conference, IEEE, 2008, pp. 1–5.
[148] S.M. Jalil, L. Abdullah, I. Ahmad, H. Abdullah, The effect of surface texturing on GaAs solar cell using TCAD tools, in: 2008 IEEE International Conference on Semiconductor Electronics, IEEE, 2008, pp. 280–283.
[149] M. Zeman, J. Krc, Optical and electrical modeling of thin-film silicon solar cells, J. Mater. Res. 23 (4) (2008) 889–898.
[150] N.E.I. Boukortt, S. Patanè, A.M. AlAmri, D. AlAjmi, K. Bulayyan, N. AlMutairi, Numerical investigation of perovskite and u-CIGS based tandem solar cells using silvaco TCAD simulation, Silicon 15 (1) (2023) 293–303.
[151] M. Okil, A. Shaker, M.M. Salah, T.M. Abdolkader, I.S. Ahmed, Investigation of polymer/Si thin film tandem solar cell using TCAD Numerical Simulation, Polymers. (Basel) 15 (9) (2023) 2049.
[152] M.S. Salem, et al., Performance Investigation of a Proposed Flipped npn Microstructure Silicon Solar Cell Using TCAD Simulation, Crystals. (Basel) 12 (7) (2022) 959.
[153] A. Li, et al., Theoretical simulation and experimental perspective of refractive index-controlled silicon nanofilms for solar cell efficiency improvement, Solar Energy Mater. Solar Cells 251 (2023) 112145.
[154] N.E.I. Boukortt, A.M. AlAmri, F. Bouhjar, K. Bouhadiba, Investigation and optimization of ultrathin Cu (In, Ga) Se 2 solar cells by using silvaco-TCAD tools, J. Mater. Sci. Mater. Electron. 32 (2021) 21525–21538.
[155] B. Dong, C.G. Bailey, A. Afanasev, M. Zaghloul, Modeling and simulation of InAs/GaAs quantum dot solar cells in SILVACO TCAD, in: 2014 IEEE 40th Photovoltaic Specialist Conference (PVSC), IEEE, 2014, pp. 0476–0478.
[156] H. Mehmood, H. Nasser, E. Özkol, T. Tauqeer, S. Hussain, R. Turan, Physical device simulation of partial dopant-free asymmetric silicon heterostructure solar cell (P-DASH) based on hole-selective molybdenum oxide (MoOx) with crystalline silicon (cSi), in: 2017 International Conference on Engineering and Technology (ICET), IEEE, 2017, pp. 1–6.
[157] M. Salem, et al., Influence of base doping level on the npn microstructure solar cell performance: A TCAD study, Opt. Mater. (Amst) 121 (2021) 111501.
[158] B. Idris, Z. Rafik, D. Kamal, B. Abdessalam, G. Faouzi, Size and grain-boundary effects on the performance of polycrystalline CIGS-based solar cells, in: IREC2015 The Sixth International Renewable Energy Congress, IEEE, 2015, pp. 1–5.
[159] N.E.I. Boukortt, B. Hadri, Simulation of electrical characteristics of PERC solar cells, J. Electron. Mater. 47 (10) (2018) 5825–5832.
[160] P. Nayak, J. Dutta, G. Mishra, Efficient InGaP/GaAs DJ solar cell with double back surface field layer, Eng. Sci. Technol. Int. J. 18 (3) (2015) 325–335.
[161] Z.A. Ansari, et al., Photovoltaic solar cells based on graphene/gallium arsenide Schottky junction, Optik. (Stuttg) 182 (2019) 500–506.
[162] S. Kashyap, J. Madan, R. Pandey, R. Sharma, Impact of phosphorus ion implantation dose on the performance of PERC solar cell, in: 2021 IEEE 48th Photovoltaic Specialists Conference (PVSC), IEEE, 2021, pp. 2247–2249.
[163] M.S. Salem, et al., Physically based analytical model of heavily doped silicon wafers based proposed solar cell microstructure, IEEe Access. 8 (2020) 138898–138906.
[164] A.Abd Rahim, et al., Investigation of light trapping mechanism of Silicon solar cell performance utilizing Silvaco TCAD, J. Phys. Confer. Ser. 1535 (1) (2020) 012021. IOP Publishing.
[165] R.A. Bakar, S.H. Herman, H. Hassan, W.R.W. Ahmad, F. Mohamad, M. M. Aminuddin, Modeling and simulation of microscopic defects in CIS-based solar cell thin film using silvaco TCAD, in: RSM 2013 IEEE Regional Symposium on Micro and Nanoelectronics, IEEE, 2013, pp. 117–121.
[166] H. Elmira, B. Dennaib, M. Fillalib, Effect of proton radiation on the performance ofInGaP/GaAs solar cell, J. Ovonic Res. Vol 17 (3) (2021) 307–311.
[167] S. Zandi, P. Saxena, M. Razaghi, N.E. Gorji, Simulation of CZTSSe thin-film solar cells in COMSOL: three-dimensional optical, electrical, and thermal models, IEEe J. Photovolt. 10 (5) (2020) 1503–1507.
[168] N. K. Das, S. F. U. Farhad, A. K. S. Gupta, M. A. Matin, and N. Amin, "The significance of bilayer window (Cds: O/Cds) on the performance of Cdte thin film solar cells," Available at SSRN 4811217.
[169] R. Abdur, et al., Enhancing perovskite solar cell performance: Investigating the impact of post-annealing on the optoelectrical and structural properties of RF-sputtered NiO films via SCAPS-1D device modeling, Solar Energy 271 (2024) 112443.
[170] P.K. Rathod, P. Solanki, B. Kataria, J. Markna, Optimisation and numerical analysis of highly efficient CGSe-based thin film solar cell, Phys. Scr. 99 (2) (2024) 025923.
[171] S. Tripathi, P. Lohia, D. Dwivedi, Contribution to sustainable and environmental friendly non-toxic CZTS solar cell with an innovative hybrid buffer layer, Solar Energy 204 (2020) 748–760.
[172] A. Kowsar et al., "A novel simulator of multijunction solar cells â€" MSCS-1D," vol. 10, no. 3, pp. 1369-1375, 2020.
[173] S. Roy, P. Bermel, Investigation of pure and hybrid tungsten-based transition metal di-chalcogenides for radiation resistant space photovoltaic applications, Opt. Mater. Express. 13 (8) (2023) 2214–2226.
[174] M.F. Ali, M.F. Hossain, M.A. Hossain, Maximizing conversion efficiency: a numerical analysis on P+ a-SiC/i interface/n-Si heterojunction solar cells with AMPS-1D, Int. J. Photoenergy 2024 (1) (2024) 6846310.
[175] Y. Shen, M. Yu, R. Huang, Q. Cheng, Numerical simulation of n-MoSe2/p-Si Solar Cells by AFORS-HET, Adv. Theory. Simul. 5 (7) (2022) 2100551.
[176] M. Zeman, J. Willemen, L. Vosteen, G. Tao, J. J. S. E. M. Metselaar, and S. Cells, "Computer modelling of current matching in a-Si: H/a-Si: H tandem solar cells on textured TCO substrates," vol. 46, no. 2, pp. 81-99, 1997.
[177] M. Vogt, et al., Introducing a comprehensive physics-based modelling framework for tandem and other PV systems, Solar Energy Mater. Solar Cells 247 (2022) 111944.
[178] F. Smole, M. Topič, and J. J. J. o. n.-c. s. Furlan, "Analysis of TCO/p (a-Si: C: H) heterojunction and its influence on pin a-Si: H solar cell performance," vol. 194, no. 3, pp. 312-318, 1996.
[179] S. Garud, M. Bokalič, C. thi Trinh, B. Rech, D. Amkreutz, M. Topič, Analysis of surface passivation and laser firing on thin-film silicon solar cells via light-beam induced current, IEEe J. Photovolt. 10 (5) (2020) 1246–1253.
[180] R. C. MacKenzie, "Gpvdm user manual v7. 88," 2022.
[181] N.S. Khairuddin, M.Z.M. Yusoff, H. Hussin, Numerical performance analysis of In0. 2Ga0. 8N/p-Si based solar cell using PC1D simulation on influence of region thicknesses, doping concentration and temperature towards power conversion efficiency (PCE), J. Optics (2024) 1–12.
[182] M. Hekmat, F. Rostamian, A. Shafiekhani, Improving solar cells characteristics by tuning the density distribution of deep trapping states using Au@ DLC decorated on photoanodes, Mater. Sci. Semicond. Process. 128 (2021) 105782.
[183] M. Shafayet-Ul-Islam, A. Kuddus, M. Kabiruzzaman, S.F.U. Farhad, A. Kowsar, Cu2FeSnS4-based heterojunction solar cells with MxOy (M= Cu, Ni)-back surface field layers: Impact of defect density states and recombination, Next Energy 6 (2025) 100196.
[184] P. Panda, S. Beriha, S.K. Tripathy, Design of MASnI3 perovskite solar cell with chalcogenide ETLs to achieve high photo conversion efficiency of 31.51% using SETFOS, Optik. (Stuttg) 296 (2024) 171550.
[185] E. Guichard, M. Eastlick, C. Hylin, A. Iontcheva, M. Roschke, State of the Art 3D SiC process and device simulatio, SILVACO (2014) [Online]. Available: https://silvaco.com/tcad/#whitepapers.
[186] Z. Seboui, S. Dabbabi, First investigation on CZTS electron affinity and thickness optimization using SILVACO-Atlas 2D simulation, Simul. Model. Pract. Theory. 126 (2023) 102758.
[187] A. Bouich et al., "Delafossite as hole transport layer a new pathway for efficient perovskite-based solar sells: Insight from experimental, DFT and numerical analysis," vol. 250, pp. 18-32, 2023.
[188] M. Mahmood, K. Sobayel, K. Noor, M.M.I. Sapeli, M.M. Hossain, M.N.E. Alam, M. A. Ibrahim, M.S. Soliman, M.T. Islam, Metal-doped perovskite oxide Ba (1-x) Sr (x) TiO3 as electron transport layer for enhanced photovoltaic performance: An FDTD study, Solar Energy 283 (2024) 112987.
[189] A. Kowsar, S.F.U. Farhad, High efficiency four junction III-V Bismide concentrator solar cell: design, theory, and simulation, Int. J. Renew. Energy Res. (IJRER) 8 (3) (2018) 1762–1769.
[190] S. Eidelloth, U. Eitner, S. Steingrube, R. Brendel, Open source graphical user interface in MATLAB for two-dimensional simulations solving the fully coupled semiconductor equations using COMSOL, in: Proc. 25th EU PVSEC, 2010, pp. 2477–2485.
[191] K.R. McIntosh, P.P. Altermatt, A freeware 1D emitter model for silicon solar cells, in: 2010 35th IEEE Photovoltaic Specialists Conference, IEEE, 2010, pp. 002188–002193.
[192] P.A. Basore, 3D numerical solutions inside the pyramid of textured silicon solar cells, in: AIP Conference Proceedings 2487, 2022.
[193] A. Fell, A free and fast three-dimensional/two-dimensional solar cell simulator featuring conductive boundary and quasi-neutrality approximations, IEEe Trans. Electron. Devices 60 (2) (2012) 733–738.
[194] A. Cuevas, Modelling silicon characterisation, Energy Proc. 8 (2011) 94–99.

[195] B. ray, C. A. G. Williamson, M. R. Khan, and M. Alam, "OPV Lab," ed, 2011.
[196] P. Saint-Cast, M. Padilla, A. Kimmerle, C. Reichel, An analytical model for interdigitated back contact solar cells, IEEe J. Photovolt. 4 (1) (2013) 114–121.
[197] D. Alonso-Álvarez, T. Wilson, P. Pearce, M. Führer, D. Farrell, N. Ekins-Daukes, Solcore: a multi-scale, Python-based library for modelling solar cells and semiconductor materials, J. Comput. Electron. 17 (2018) 1099–1123.
[198] S.Ould Saad Hamady, Solis: a modular, portable, and high-performance 1D semiconductor device simulator, J. Comput. Electron. 19 (2) (2020) 640–647.