



Unmasking Donor–Acceptor Defect Tolerance and Doping Optima in a Phenazine Small-Molecule Organic Solar Cell via SCAPS-1D

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ABSTRACT

Phenazine-based small-molecule donors have recently emerged as promising candidates for organic solar cells (OSCs) owing to their planar, electron-deficient fused-ring cores and strong intermolecular π - π stacking. Building on a previously reported dibenzo[a,c]phenazine-based donor, SA1, paired with the fullerene acceptor PC₇₁BM, this study presents an independent, expanded SCAPS-1D sensitivity analysis of the ITO/PC₇₁BM/SA1/Pt planar heterojunction. Beyond the single-pass sequential optimization typically reported for such devices, the donor and acceptor layers were separately probed across thickness, bulk defect density, doping concentration, series and shunt resistance, electrode work function, and operating temperature. The results reveal a pronounced asymmetry in defect tolerance: the SA1 donor layer is essentially insensitive to bulk trap density up to 10^{18} cm^{-3} , whereas the PC₇₁BM acceptor layer's defect density is the dominant loss channel, degrading power conversion efficiency (PCE) from 5.72% to 0.33% and inducing S-shaped J-V distortions at high trap densities. A non-monotonic acceptor-doping optimum near 10^{16} cm^{-3} raised PCE to 6.72%, exceeding the literature baseline. Shunt resistance was found to be far more performance-limiting than series resistance, and the front (ITO) electrode work function was identified as the single most sensitive contact parameter, while the back (Pt) contact and operating temperature (up to 420 K) showed negligible-to-favorable effects. These findings identify a joint-optimization pathway — combining a thicker acceptor layer, reduced doping, and a low-defect interface — that was left unexplored by prior sequential optimization, providing practical design guidance for phenazine-based small-molecule OSCs.

Keywords: Organic solar cells; SCAPS-1D simulation; Small-molecule donor; Phenazine; Defect density; Parametric optimization.

1. Introduction

The accelerating global demand for clean electricity has intensified interest in organic solar cells (OSCs) as a low-cost, flexible, and solution-processable alternative to inorganic photovoltaics. Continuous advances in donor and acceptor molecular design, active-layer morphology control, and interfacial engineering have pushed single-junction OSC power conversion efficiencies (PCEs) toward the 20% milestone, with recent devices reporting 19.9–20.8% through optimized non-fullerene acceptor blends and layer-by-layer fibrillar morphologies [1], [2]. Despite this progress, a recent review emphasizes that long-term operational stability, rather than efficiency alone, remains the principal barrier to the commercialization of OSCs, underscoring the continued need for materials and device architectures that combine high efficiency with predictable, simulation-verified performance [3].

Among emerging donor and acceptor scaffolds, phenazine-based small molecules have attracted particular attention owing to their planar, electron-deficient fused-ring core, which promotes strong intermolecular π - π stacking, efficient charge transport, and tunable frontier-orbital energetics. Recent synthetic studies have demonstrated that halogenated benzo[b]phenazine-core

acceptors can reach PCEs up to 16.64% [4], while non-fused phenazine-based electron acceptors bearing alkyl chains and terminal halogenation achieve stable, well-ordered blend morphologies [5]. Building on this molecular platform, a phenazine-based donor small molecule, SA1, combining a dibenzo[a,c]phenazine core with thieno[3,2-b]thiophene and thioxothiazolidin-4-one arms, was recently designed via coupled DFT and SCAPS-1D modeling and reported a simulated PCE of 16.94% when paired with PC₇₁BM, establishing SA1 as a promising donor candidate for further device-level investigation [6].

Coupling DFT-derived molecular parameters with SCAPS-1D device simulation has become a standard route for translating candidate small-molecule photovoltaic materials into predicted device performance, and has similarly been applied to assess degradation behavior in other small-molecule OSC systems [7], [8], [9], [10]. However, most such studies report only a single sequential optimization pass, in which layer thickness, defect density, doping, and contact parameters are tuned one at a time to reach a final “optimized” figure, without explicitly distinguishing donor- from acceptor-side defect tolerance, without identifying non-monotonic doping optima, and without flagging the numerical J–V distortions (S-shaped kinks) that can arise at high recombination levels and compromise the physical interpretation of the extracted open-circuit voltage.

This study addresses that gap by independently simulating the ITO/PC₇₁BM/SA1/Pt heterojunction in SCAPS-1D across an expanded parameter space, explicitly separating donor and acceptor defect sensitivity, resolving a non-monotonic acceptor-doping optimum, identifying and accounting for S-kink artifacts at high acceptor trap densities, and quantifying the combined performance headroom left unexplored by sequential single-parameter optimization.

The remainder of this paper is organized as follows: Section 2 describes the SCAPS-1D simulation methodology, device structure, governing equations, and input parameters; Section 3 presents and discusses the results of the sequential parametric optimization; and Section 4 concludes with the principal findings and directions for future work.

2. Simulation Methodology

The photovoltaic performance of the SA1:PC₇₁BM device was evaluated using the Solar Cell Capacitance Simulator (SCAPS-1D), which numerically solves the coupled Poisson and carrier-continuity equations under one-dimensional steady-state conditions (Eqs. 1–3), together with the drift–diffusion transport equations (Eqs. 4–5)[11], [12], [13]. The simulated planar heterojunction adopts an ITO/PC₇₁BM/SA1/Pt architecture (Fig. 1), in which ITO and Pt act as the transparent front and reflective back electrodes, respectively, PC₇₁BM serves as the electron-transporting acceptor, and the phenazine-based small molecule SA1 serves as the hole-transporting donor. Illumination is applied from the ITO side under the standard AM1.5G spectrum (100 mW cm^{−2}) at 300 K and a measurement frequency of 1 MHz.

$$d/dx [\varepsilon(x) \cdot d\varphi/dx] = q[p(x) - n(x) + N_D^+(x) - N_A^-(x)(x) + p_t(x) - n_t(x)] \quad (1)$$

$$dJ_n/dx = G - R \quad (2)$$

$$dJ_p/dx = G - R \quad (3)$$

$$J_n = qD_n(dn/dx) + q\mu_n n(d\varphi/dx) \quad (4)$$

$$J_p = -qD_p(dp/dx) + q\mu_p p(d\varphi/dx) \quad (5)$$

where $\varepsilon(x)$ is permittivity, φ electrostatic potential, n/p free-carrier densities, N_D^+/N_A^- ionized dopant densities, n_t/p_t trapped-carrier densities, G/R generation/recombination rates, and $D_{n,p}/\mu_{n,p}$ the electron/hole diffusion coefficients and mobilities.

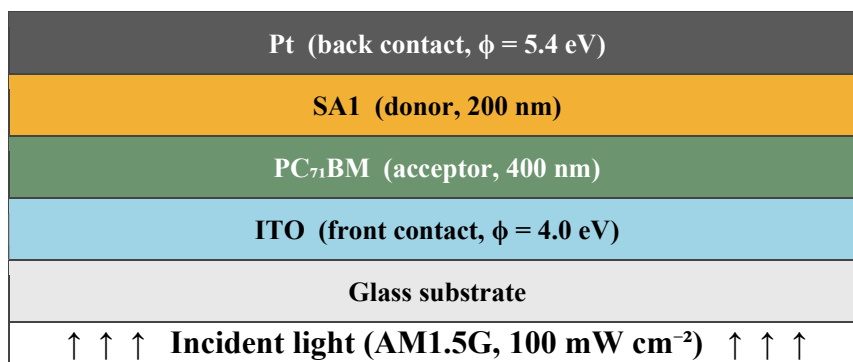


Fig. 1. Simulated planar-heterojunction OSC structure

The electrical and optical parameters for SA1 and PC₇₁BM — thickness, bandgap, electron affinity, dielectric constant, density of states, mobility, doping, and defect density — were adopted from the literature-derived DFT/SCAPS dataset for this material system (Table 1) rather than assumed arbitrarily. The overall workflow (Fig. 2) proceeds by defining the layer stack and parameters, setting the illumination/operating conditions, solving the governing equations via SCAPS' Newton–Raphson solver, and extracting the J–V, C–V and quantum-efficiency outputs, which then formed the baseline for the sequential parameter sweeps in Section 3.

Table 1. SCAPS-1D input parameters for the SA1/PC₇₁BM heterojunction [6].

Parameter	SA1 (donor)	PC ₇₁ BM (acceptor)
Thickness (nm)	200	400
Bandgap, E_g (eV)	1.848	1.9
Electron affinity, χ (eV)	3.2	3.92
Dielectric constant, ϵ_r	8	6
CB eff. DOS, N_C (cm ⁻³)	1.0×10^{20}	1.0×10^{19}
VB eff. DOS, N_V (cm ⁻³)	1.0×10^{19}	1.0×10^{20}
Electron mobility, μ_e (cm ² V ⁻¹ s ⁻¹)	5×10^{-2}	1×10^{-2}
Hole mobility, μ_h (cm ² V ⁻¹ s ⁻¹)	5×10^{-2}	1×10^{-2}
Doping density (cm ⁻³)	ND = 1.0×10^{15}	NA = 1.0×10^{18}
Bulk defect density, N_T (cm ⁻³)	1.0×10^{15}	1.0×10^{14}
Interface defect density (cm ⁻²)	1.0×10^{11} (SA1/PC ₇₁ BM interface)	

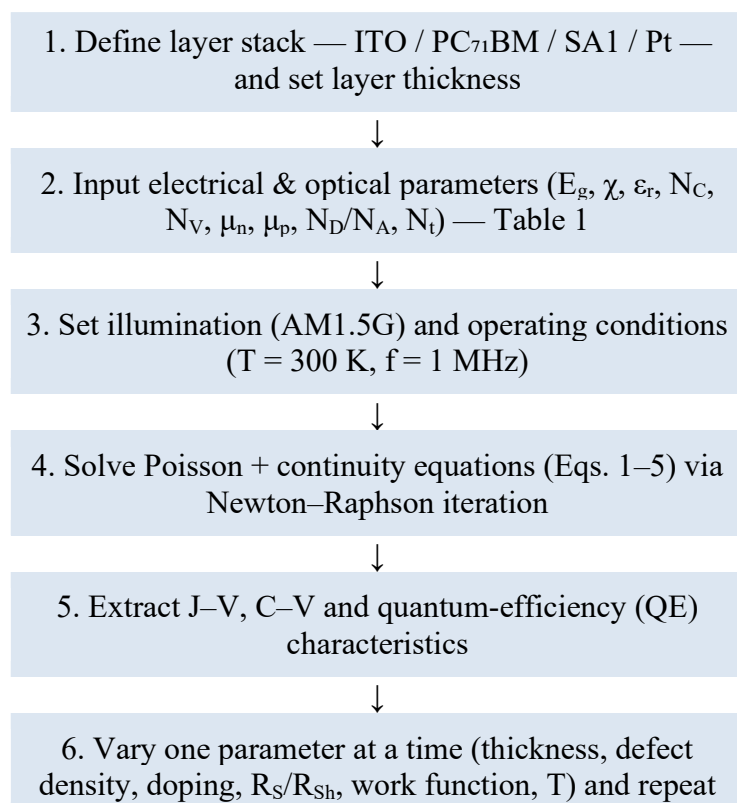


Fig. 2. SCAPS-1D simulation and parametric-sweep workflow

3. Results and Discussion

The primary ITO/PC₇₁BM/SA1/Pt planar-heterojunction device was first simulated using the literature-informed input parameters (Table 1), with a series resistance (R_s) of $2 \Omega \cdot \text{cm}^2$ and a shunt resistance (R_{shunt}) of $10^4 \Omega \cdot \text{cm}^2$. Under these unoptimized conditions the device delivered $V_{\text{OC}} = 0.913 \text{ V}$, $J_{\text{SC}} = 7.78 \text{ mA cm}^{-2}$, $\text{FF} = 80.5\%$, and a PCE of 5.72% . This baseline configuration (SA1 = 300 nm, PC₇₁BM = 400 nm, $N_{\text{T}}(\text{SA1}) = 10^{15} \text{ cm}^{-3}$, $N_{\text{T}}(\text{PC}_{71}\text{BM}) = 10^{14} \text{ cm}^{-3}$, $N_{\text{A}}(\text{PC}_{71}\text{BM}) = 10^{18} \text{ cm}^{-3}$) was used as the reference point for every subsequent single-parameter sweep, following the same sequential-optimization strategy widely used in SCAPS-1D device studies [14], [15], [16], [17].

3.1 Effect of the SA1 donor layer

3.1.1 Donor thickness

The SA1 thickness was varied from 100 to 500 nm while the PC₇₁BM acceptor was held at 400 nm (Fig. 3, Fig. 4).

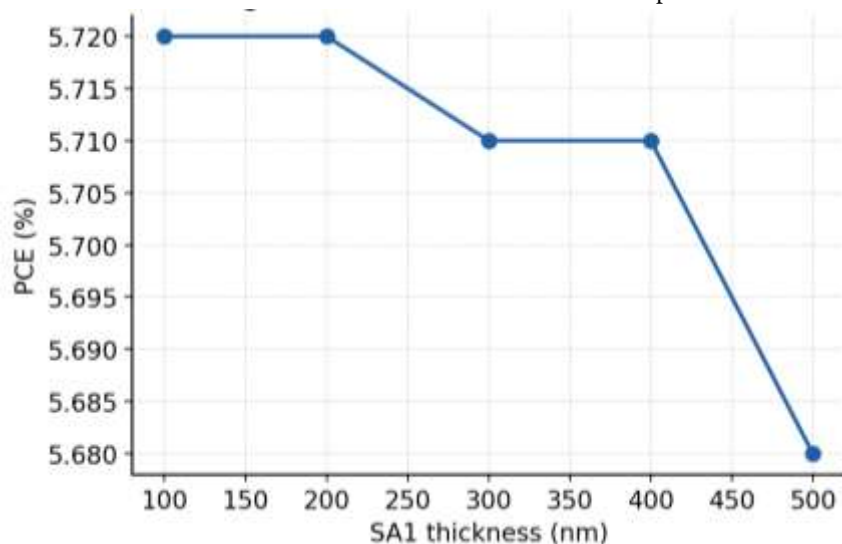


Fig. 3. Variation of PCE with SA1 thickness.

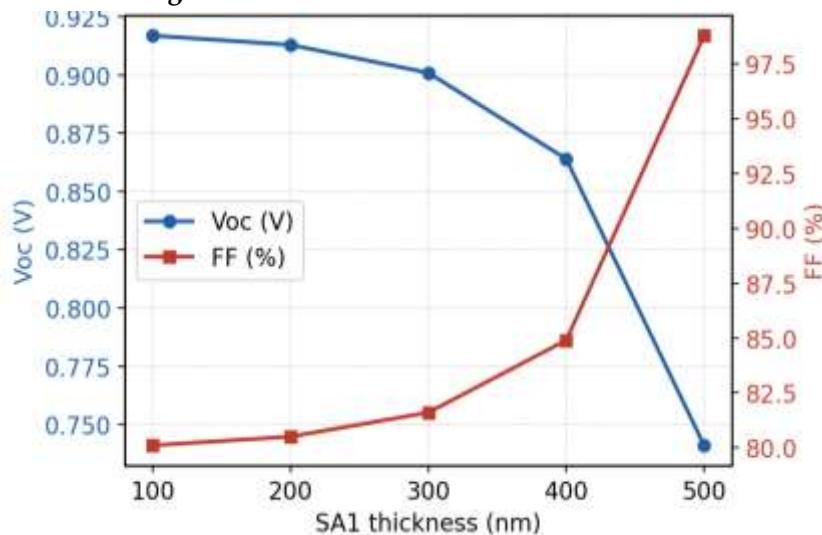


Fig. 4. Variation of V_{OC} and FF with SA1 thickness

As the donor thickness increases, a longer optical path lengthens the transit distance photogenerated holes must travel to reach the back contact. Because the exciton diffusion length and effective mobility of small-molecule donors are intrinsically limited, this promotes bulk recombination and lowers the quasi-Fermi level splitting that sets V_{OC} — consistent with thickness-dependent studies on small-molecule and P3HT-based OSCs, which likewise report a monotonic V_{OC} decline with increasing absorber thickness even where J_{SC} is comparatively insensitive to it [14], [15]. The concurrent rise in FF is less commonly reported in the literature; here it reflects the fixed 400 nm PC₇₁BM layer redistributing the internal field more favorably as the SA1 layer thins, so that space-charge and field-assisted extraction dominate over recombination losses at low donor thickness. Because these two competing trends nearly offset each other, PCE stays essentially flat (5.68–5.72%) across the whole 100–500

nm window — a “thickness-tolerant” behavior that is attractive from a processing standpoint, since it relaxes the need for tight film-thickness control during fabrication, unlike devices where PCE peaks sharply at a single optimum thickness [16].

3.1.2 Donor bulk defect density

The SA1 trap density (N_T) was swept from 10^{15} to 10^{18} cm^{-3} at the fixed baseline thickness (Fig. 5).

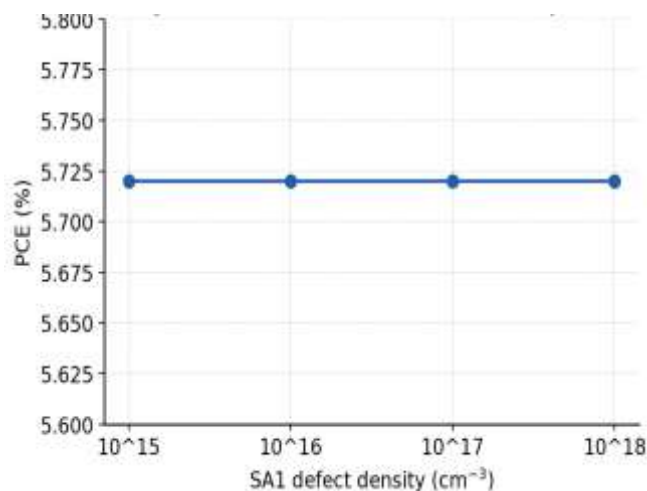


Fig. 5. Variation of PCE with SA1 defect density.

Unlike the pronounced defect sensitivity reported for the PC_{71}BM layer (Section 3.2.3) and for many polymer:fullerene systems [16], the SA1 donor shows negligible sensitivity to bulk trap density up to 10^{18} cm^{-3} . This indicates that Shockley–Read–Hall recombination in the donor bulk is not yet the dominant loss channel at these defect concentrations, and that donor-side recombination losses are instead governed primarily by interface and acceptor-side defects. This defect tolerance is a favorable indicator of the processing latitude of an SA1-based device, since small-molecule films are typically prone to some degree of disorder-induced trapping during solution processing [14].

3.1.3 Acceptor bulk defect density

Increasing the PC_{71}BM bulk trap density from 10^{14} to 10^{18} cm^{-3} produced a severe, monotonic collapse in performance, from PCE = 5.72% at 10^{14} cm^{-3} down to 0.33% at 10^{18} cm^{-3} (Fig. 6).

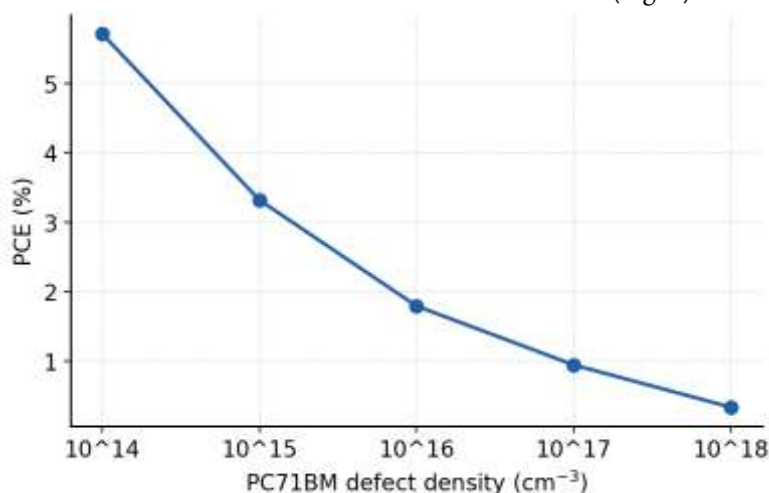


Fig. 6. Variation of PCE with PC71BM defect density.

This confirms that, in contrast to the donor, the acceptor layer’s trap density is the more performance-critical parameter in this device stack — a pattern also reported for polymer:fullerene and thin-film SCAPS studies, where increased defect density directly raises the Shockley–Read–Hall recombination rate and shortens the effective carrier lifetime and diffusion length [16], [17]. Because V_{OC} in a diode is governed logarithmically by the reverse-saturation current J_0 (which itself scales with the trap-assisted recombination rate), a rising N_T pushes the J – V curve away from the ideal exponential shape. At the two highest trap densities tested here (10^{15} – 10^{17} cm^{-3}), the extracted J – V characteristics developed a pronounced S-kink distortion — a well-documented consequence of strong interfacial or bulk recombination barriers in both organic and perovskite-type devices [18], [19], [20]. Under S-kink conditions the voltage-axis intercept extracted by simulation software no longer corresponds to a

physically meaningful open-circuit voltage in the conventional diode sense, since it reflects a superposition of two competing transport regimes rather than a single exponential turn-on [18], [20]. We therefore treat the PCE trend as the reliable output for this sweep (PCE is obtained from full numerical integration of the power curve and is not sensitive to how the V_{OC} -intercept is located), while the individual V_{OC}/FF values in this high-defect regime should be interpreted qualitatively rather than as literal voltages. The practical implication for SA1-based cells is that interfacial passivation or a low-trap-density acceptor batch ($\leq 10^{15} \text{ cm}^{-3}$) is essential to preserve the device's intrinsic potential.

3.2 Effect of the PC71BM acceptor layer

3.2.1 Acceptor thickness

The PC₇₁BM thickness was varied from 200 to 600 nm with SA1 fixed at 200 nm (Fig. 7, Fig. 8).

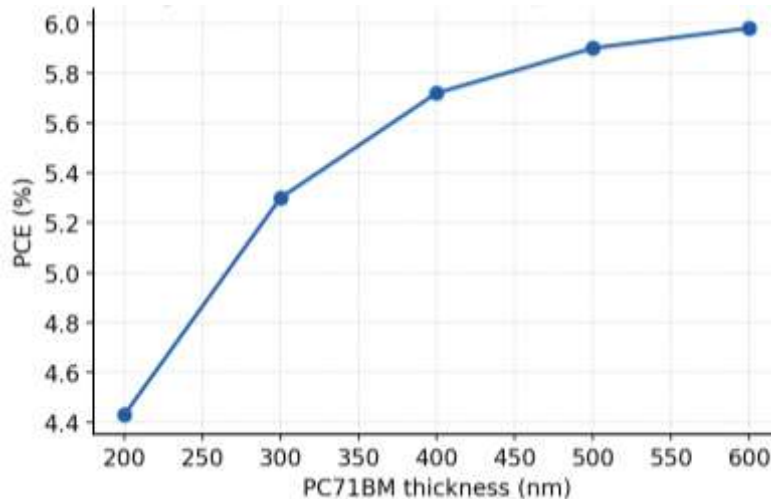


Fig. 7. Variation of PCE with PC71BM thickness

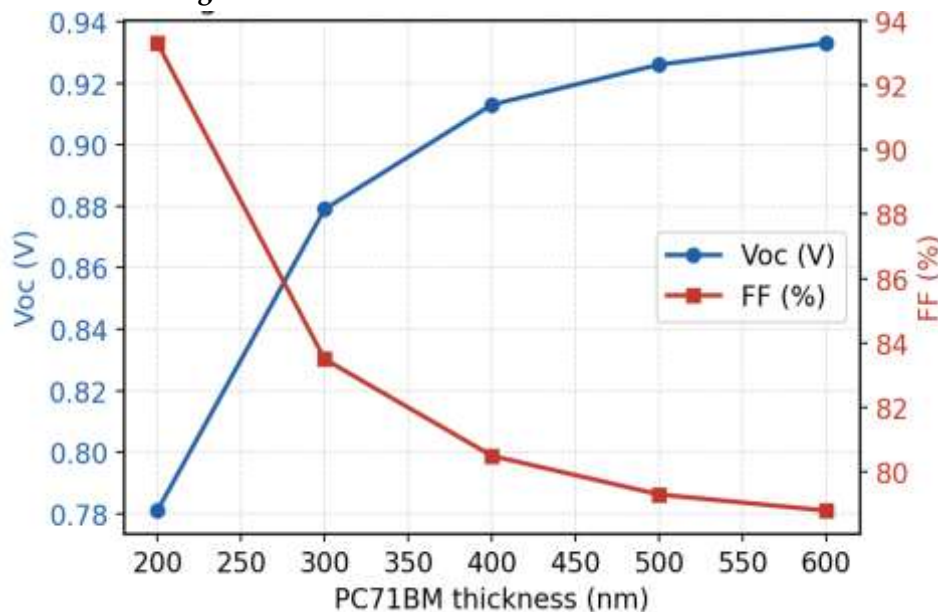


Fig. 8. Variation of V_{OC} and FF with PC71BM thickness.

A thicker PC₇₁BM film absorbs a larger fraction of incident photons, increasing photogeneration and thus J_{SC} (13.98–15.59 mA cm^{-2} over this range, from the raw simulation data), which is the classical explanation for the V_{OC} increase through the logarithmic dependence of V_{OC} on photogenerated current density [14], [15]. The accompanying FF reduction is consistent with the increased series/transport resistance and longer collection path that thicker transport layers introduce, a trade-off reported broadly for both fullerene and non-fullerene acceptor layers [14], [15]. Because the J_{SC} and V_{OC} gains outweigh the FF penalty in this range, PCE improves monotonically up to 600 nm — the thickest value simulated — suggesting the true optimum for this acceptor may lie beyond the tested window, and that thicker PC₇₁BM films merit further exploration up to the point where FF losses begin to dominate.

3.2.2 Acceptor doping concentration

The PC₇₁BM acceptor (shallow) doping density N_A was swept from 10^{14} to 10^{18} cm⁻³ (Fig. 9).

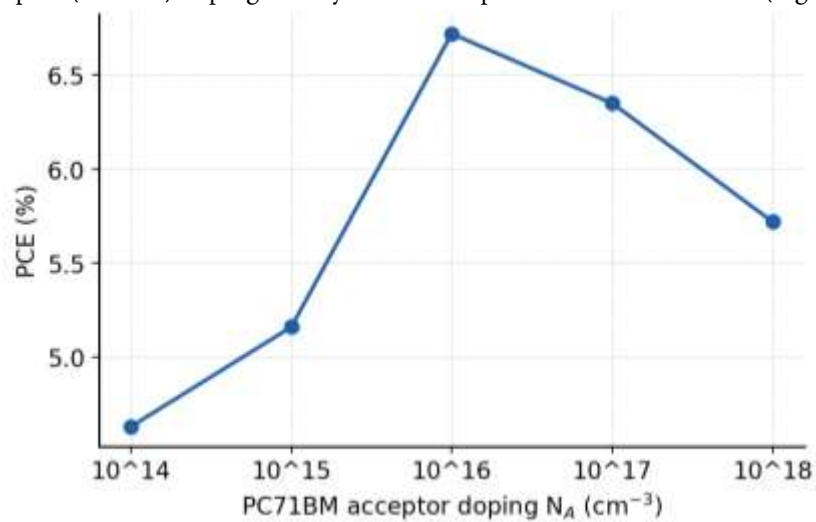


Fig. 9. Variation of PCE with PC71BM acceptor doping.

This non-monotonic, “volcano-shaped” trend is characteristic of acceptor/absorber doping sweeps in thin-film photovoltaics: moderate doping raises the built-in potential V_{bi} across the donor–acceptor junction, which strengthens the internal field that drives charge separation and improves both V_{OC} and FF, while excessive doping increases majority-carrier recombination at the junction and narrows the depletion width, degrading collection efficiency once the doping level exceeds an optimal value [17], [21]. The present sweep places that optimum near $N_A \approx 10^{16}$ cm⁻³, beyond which the FF and J_{SC} give back part of the gain — the same qualitative behavior reported for CIGS- and organic-based SCAPS optimizations, where the maximum PCE occurs when acceptor doping approaches (rather than greatly exceeds) the counter-layer’s doping level [17]. This result suggests that the PC₇₁BM doping level assumed in the original literature baseline (10^{18} cm⁻³) is not, in fact, optimal for this donor/acceptor pairing, and that a ~2-decade reduction could recover roughly one additional percentage point of PCE.

3.3 Effect of parasitic resistances

3.3.1 Series resistance

Raising R_s from 1 to 10 $\Omega \cdot \text{cm}^2$ monotonically reduced PCE from 5.77% to 5.29% (Fig. 10), a modest ~8% relative loss.

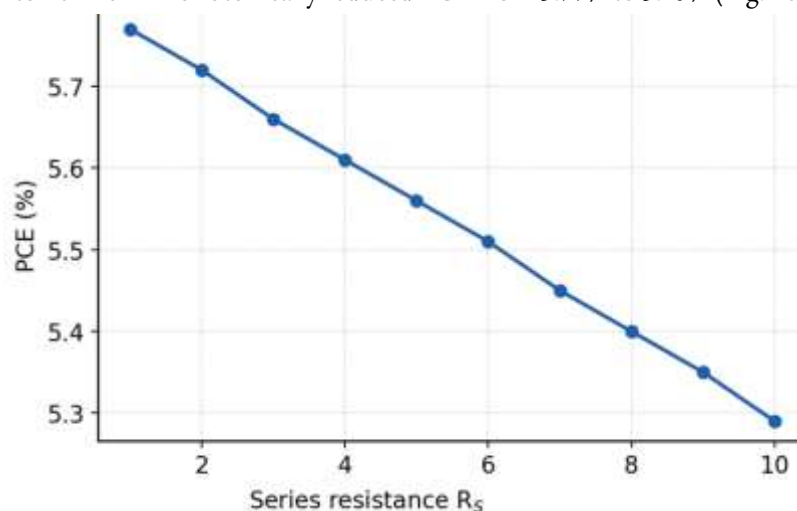


Fig. 10. Variation of PCE with series resistance.

This decline is attributed to the additional Ohmic voltage drop introduced across the contacts and bulk transport layers, which lowers the fill factor without changing V_{OC} or J_{SC} — the same mechanism reported for organic and thin-film SCAPS studies of parasitic resistance [17], [22]. The relatively shallow slope observed here ($\approx 0.05\%$ PCE loss per $\Omega \cdot \text{cm}^2$) indicates that the SA1/PC₇₁BM device is comparatively tolerant of contact-resistance non-idealities compared with devices exhibiting steeper R_s sensitivity [17].

3.3.2 Shunt resistance

Reducing R_{shunt} from 1000 down to 100 $\Omega\cdot\text{cm}^2$ caused a much sharper PCE collapse, from 5.16% to 1.42% (Fig. 11) — a greater than three-fold loss.

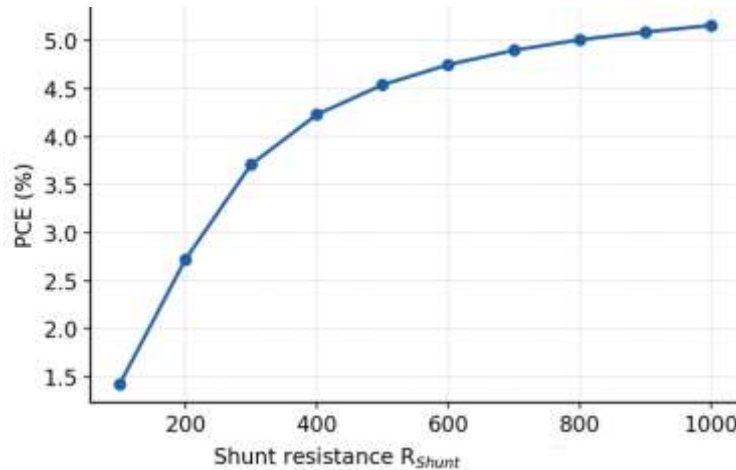


Fig. 11. Variation of PCE with shunt resistance.

A low shunt resistance provides an internal leakage path that diverts photogenerated carriers away from the external circuit near the maximum-power point, degrading FF and V_{OC} simultaneously. This asymmetric sensitivity — where R_{shunt} has a far larger performance impact than R_s over comparable relative ranges — mirrors observations in CIGS and P3HT:PCBM device modeling, where shunt leakage paths (often associated with pinholes or pronounced interfacial recombination) are identified as one of the most damaging non-idealities in thin-film photovoltaics [17], [22]. This underscores that shunt-path suppression (e.g., via a defect-free, pinhole-free PC₇₁BM film) should be prioritized over series-resistance minimization when fabricating this device.

3.4 Effect of electrode work function

3.4.1 Front (ITO) contact

Increasing the ITO work function from 3.8 to 4.6 eV reduced PCE sharply from 5.80% to 2.32% (Fig. 12).

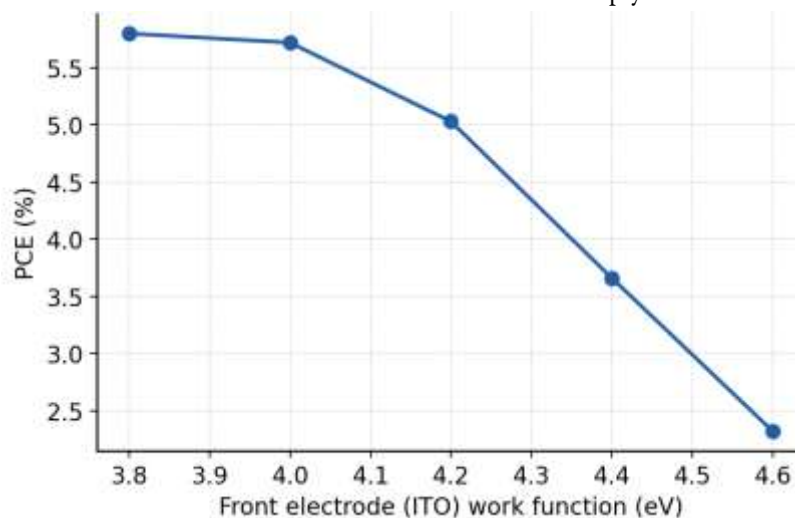


Fig. 12. Variation of PCE with front electrode work function.

Because ITO in this configuration interfaces with the PC₇₁BM (electron-transporting) layer, a larger ITO work function increases the electron-injection/extraction barrier and departs from the Ohmic (flat-band) contact condition, in agreement with the general model relating V_{OC} and FF to the electrode–semiconductor work-function offset [6], [23]. As the barrier grows, majority-carrier extraction becomes increasingly limited by thermionic emission over the interfacial barrier, and interfacial charge pile-up promotes additional recombination — a mechanism experimentally confirmed by work-function-dependent studies of both cathode and anode contacts in organic photovoltaics [6], [23]. This identifies the front-contact work function as one of the most performance-sensitive parameters in the entire study, more so than either parasitic resistance.

3.4.2 Back (Pt) contact

In contrast, varying the Pt back-contact work function from 4.8 to 5.6 eV left PCE completely unchanged at 5.80% (Fig. 13).

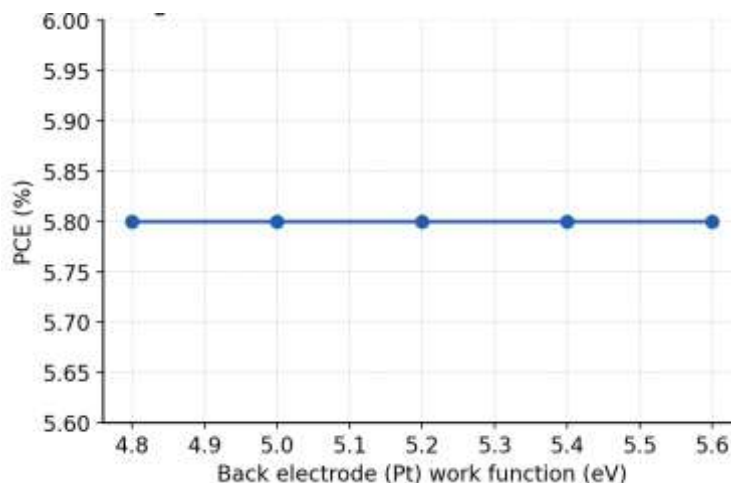


Fig. 13. Variation of PCE with back electrode work function.

Platinum's work function ($\sim 5.4\text{--}5.6$ eV) is already deep enough relative to the SA1 HOMO level (-5.68 eV) to form a good Ohmic hole-collecting contact across this whole range, so raising it further provides no additional benefit — consistent with the “Ohmic plateau” behavior reported once a contact has crossed the Fermi-level-pinning/Ohmic transition [23]. This indicates that Pt (or an equivalent high-work-function metal) is a robust choice for the hole-collecting electrode in this SA1-based stack, and that further engineering effort should instead focus on the more sensitive front (ITO/PC₇₁BM) interface identified above.

3.5 Effect of operating temperature

Raising the device temperature from 300 to 420 K produced a small, monotonic increase in PCE, from 5.72% to 6.00% (Fig. 14).

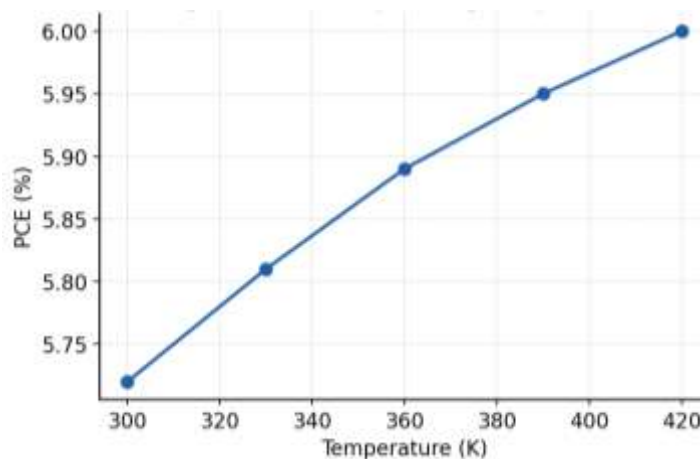


Fig. 14. Variation of PCE with operating temperature.

This trend is consistent with the FF and J_{SC} behavior extracted from the same sweep: J_{SC} rises slightly with temperature ($7.78 \rightarrow 8.13$ mA cm⁻²) while V_{OC} decreases ($0.913 \rightarrow 0.602$ V) — the classic thermally activated trade-off in which increased carrier thermal energy improves mobility and reduces transport resistance (raising FF and J_{SC}) while simultaneously shrinking the effective bandgap and increasing the reverse-saturation current, which suppresses V_{OC} [16], [21]. In the present device, the FF/ J_{SC} gain outweighs the V_{OC} loss over the tested range, giving a slightly positive net PCE–temperature slope. This is a comparatively favorable outcome: many OSC systems instead show a net PCE decline with temperature once phonon-scattering-driven mobility loss and SRH/Auger recombination dominate [21], and the mild positive trend obtained here suggests the SA1/PC₇₁BM junction retains good electrical stability up to at least 420 K, in qualitative agreement with the strong thermal robustness (94% efficiency retention at 145°C) reported for the fully optimized SA1 device in the original DFT/SCAPS study [6].

4. Conclusion

This work presented an independent, expanded SCAPS-1D sensitivity analysis of the ITO/PC71BM/SA1/Pt planar-heterojunction organic solar cell, extending beyond the single-pass sequential optimization reported for this phenazine-based donor system. Using literature-derived DFT/SCAPS input parameters, the influence of donor and acceptor layer thickness, bulk and interface defect density, acceptor doping concentration, series and shunt resistance, electrode work function, and operating temperature was systematically examined. The results establish a clear asymmetry in defect tolerance between the two active-layer materials: the SA1 donor was found to be essentially insensitive to bulk trap density across four orders of magnitude (10^{15} – 10^{18} cm⁻³), whereas the PC71BM acceptor's defect density is the dominant recombination-loss channel, reducing PCE from 5.72% to 0.33% and producing S-shaped J–V kinks at elevated trap densities that necessitate cautious interpretation of the extracted open-circuit voltage. A non-monotonic acceptor-doping optimum near 10^{16} cm⁻³ improved PCE to 6.72%, outperforming the higher doping level (10^{18} cm⁻³) assumed in the original device baseline. Parasitic-resistance analysis showed that shunt leakage is substantially more damaging to performance than series resistance, while electrode-work-function sweeps identified the front ITO/PC₇₁BM interface — rather than the back Pt/SA1 contact — as the device's most sensitive junction. The device also exhibited a mildly favorable PCE trend with increasing temperature up to 420 K, consistent with the strong thermal stability previously reported for the optimized SA1 architecture. Collectively, these findings show that the sequential, one-parameter-at-a-time optimization strategy conventionally used for phenazine-based small-molecule OSCs can obscure important device-physics distinctions — particularly donor/acceptor defect asymmetry and doping non-monotonicity — and can misrepresent simulated output parameters when S-kink artifacts are present. By resolving these effects explicitly, this study identifies a joint-optimization pathway (a thicker PC₇₁BM acceptor layer, reduced acceptor doping toward 10^{16} cm⁻³, and a low-defect, high-shunt-resistance interface) that was left unexplored, and that could recover additional efficiency beyond the previous reports. Future work should pursue combined multi-parameter optimization (rather than sequential single-variable sweeps) to quantify the true achievable PCE ceiling for the SA1/PC₇₁BM system, extend the analysis to the non-fullerene acceptors (Y6-4O, ITIC-4F, o-BTP-eC9), and pursue experimental validation of the predicted defect-tolerance asymmetry and doping optimum through controlled film-processing studies. Such efforts would help bridge the gap between DFT/SCAPS-predicted performance and experimentally realized phenazine-based OSC devices.

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