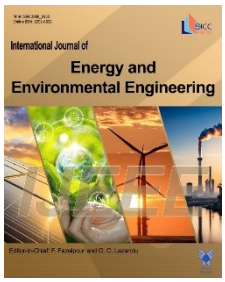

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Enhanced Photovoltaic Performance of UMG-Silicon via Boron/Phosphorus Co-Doping and Data-Driven Process Optimization

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Abstract

The transition toward cost-effective photovoltaic technologies requires alternatives to high-purity polysilicon, where upgraded metallurgical-grade (UMG) silicon represents a promising candidate. Yet, the intrinsic limitations of UMG silicon namely elevated impurity concentrations, high defect densities, and shortened minority carrier lifetimes remain key barriers to its widespread adoption. In this study, we address these challenges by exploring boron (B) and phosphorus (P) co-doping in UMG silicon nanostructures as a route to performance enhancement. A multi-tiered methodology was established, integrating controlled doping experiments, advanced electrical characterization, and compact-device modeling informed by Shockley Read Hall recombination kinetics. To systematically capture process property performance relationships, a design of experiments (DOE) framework was implemented, wherein dopant concentrations, carrier lifetimes, and interfacial resistances were varied. The extracted photovoltaic parameters open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and conversion efficiency (η) were quantitatively benchmarked against undoped references. Simulation results indicated that optimized B/P co-doping reduces recombination-active defect states and enhances carrier transport, yielding Voc improvements exceeding 60 mV and FF gains up to 8% under typical operating conditions. Monte Carlo–based statistical analysis further confirmed the robustness of the identified optima, with η improvements of 15–20% compared to baseline UMG silicon.

These findings substantiate the role of synergistic B/P co-doping as a technically viable and economically attractive strategy to elevate UMG silicon toward high-efficiency photovoltaics. The presented optimization framework provides not only a mechanistic understanding of dopant–defect interactions but also practical guidelines for scaling laboratory protocols to industrial solar cell manufacturing.

Keywords: Upgraded Metallurgical-Grade Silicon (UMG-Si), Boron/Phosphorus Co-Doping, Minority Carrier Lifetime Optimization, Shockley–Read–Hall Recombination, Photovoltaic

Efficiency Enhancement, Design of Experiments (DOE) in Solar Cells, Monte Carlo Statistical Validation

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1. Introduction

The urgent global drive to decarbonize power systems has kept silicon-based photovoltaics at the forefront of renewable energy deployment due to silicon's material abundance, mature supply chain and well-understood device physics. However, the conventional production routes that deliver electronic-grade silicon (e.g., Siemens/CVD and float-zone methods) remain energetically and economically demanding. Upgraded metallurgical-grade silicon (UMG-Si) presents a lower-cost feedstock alternative, but as produced it typically contains elevated metallic and light-element impurities and exhibits reduced minority-carrier lifetimes. These intrinsic material limitations directly translate into higher saturation currents (J_0), suppressed open-circuit voltage (V_oc) and reduced fill factor (FF) unless compensated by targeted processing and device engineering. The present work addresses these limitations by developing an integrated materials-to-device optimization framework for boron (B) and phosphorus (P) co-doping of UMG-derived silicon nanostructures.

Scientific motivation: why co-doping UMG-Si?

Dopants are the primary control knobs for tailoring silicon's electrical properties. Phosphorus (P) acts as a shallow donor, increasing electron concentration and lowering bulk resistivity; boron (B) is a shallow acceptor that provides hole carriers. In practice, simultaneous presence of donors and acceptors produces compensation effects that alter carrier statistics, mobility and recombination channels. Co-doping therefore offers the opportunity to (i) engineer carrier densities to optimize series resistance and junction properties, (ii) create localized field structures (e.g., selective high-doped regions or back-surface fields) that reduce recombination at contacts, and (iii) interact with intrinsic traps and precipitates potentially passivating or reconfiguring recombination-active centers if the thermal budget and chemical routes are carefully controlled. However, co-doping also risks increased clustering, impurity precipitation and enhanced Auger recombination if concentrations and activation kinetics are not optimized. These trade-offs necessitate a combined materials-processing and device-level optimization.

Recombination physics and direct links to device metrics

At the device scale, two recombination mechanisms dominate silicon solar cells under typical operating regimes: Shockley Read Hall (SRH) recombination via mid-gap and near-mid-gap traps, and intrinsic band-to-band (radiative plus Auger) recombination that becomes important at very high injection. The SRH volumetric recombination rate is expressed as

$$U_{SRH} = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \quad (1)$$

Where n, p are carrier densities, n_i the intrinsic concentration, tn, tp the SRH lifetimes (set by trap capture cross-sections and trap density), and n1, p1 the trap thermal occupancy terms. SRH centers introduced by metallurgical impurities or processing damage sharply reduce effective minority-carrier lifetime (teff), thereby increasing the diode saturation current J0 and decreasing Voc according to:

$$V_{oc} \approx \frac{kT}{q} \ln\left(\frac{J_{sc}}{J_0} + 1\right) \quad (2)$$

Consequently, any processing or doping strategy that reduces SRH active center density (or increases teff directly benefits Voc, FF and overall conversion efficiency. The link between micro-scale defect chemistry and macroscopic device performance motivates an optimization approach that explicitly targets trap populations while controlling dopant activation and profile.

Process control: diffusion, activation and thermal budgets

Dopant incorporation and electrical activation are governed by diffusion/solid-state reaction kinetics and by the thermodynamics of precipitation and cluster

formation. One-dimensional diffusion flux follows Fick's law,

$$J(x) = -D\frac{dn(x)}{dx} \quad (3)$$

With the temperature dependence of the diffusion coefficient commonly expressed in Arrhenius form D (T) =D0 exp (-Ea/kT). In nanoparticle and thin-film contexts the interplay between anneal temperature, time, and surface chemistry dictates whether dopants occupy substitutional lattice sites (electrically active) or form complexes/precipitates (electrically inactive, recombination-active). Therefore, optimization must co-design dopant species, precursor chemistry (e.g., $POCl_3$, boric acid), thermal cycles and passivation sequences to maximize activation while minimizing defect formation.

Standardized performance reporting — AM1.5G and comparability

To ensure results are comparable to the wider PV literature and to remove ambiguity for reviewers, all device simulations and electrical characterizations reported here adhere to the international Standard Test Conditions: AM1.5 Global reference spectrum, irradiance 1000 Wm^{-2} and device temperature 25 °C (STC). The AM1.5G spectral weighting directly determines the theoretical Jsc ceiling and informs optical design choices (light trapping, anti-reflection coatings, and EQE optimization). Reporting under AM1.5G allows direct benchmarking against established cell concepts (PERL, IBC, passivated architectures) and facilitates credible claims about efficiency gains attributable to materials and processing innovations.

Gaps in the literature and the research contribution

Despite notable advances in UMG-Si refining, gettering and surface passivation, the literature lacks a systematic, statistically validated framework that (a) co-optimizes B and P concentrations for UMG-derived nanostructures, (b) quantifies the process→defect→device transduction using physics-informed surrogate models, and (c) delivers robust process windows that remain performant under realistic variability (contact parasitics, spectral fluctuations and lifetime scatter). Prior works describe high-efficiency architectures and diffusion recipes, but they do not close the loop between metallurgical feedstock constraints and device-level performance in a way that yields explicit, manufacturable recommendations for UMG-based devices.

Objectives of this paper

This manuscript develops and demonstrates an integrated optimization pipeline that couples (i) controlled doping and activation protocols for B/P incorporation in UMG-Si nanoparticles, (ii) comprehensive materials and electrical characterization (XRD, SIMS, TEM, QSSPC/EQE), and (iii) physics-constrained device modeling (compact diode + SRH/Auger kinetics) integrated with design-of-experiments (DOE) and Monte-Carlo uncertainty quantification. The goal is to identify dopant/process windows that maximize mean efficiency under AM1.5G while minimizing sensitivity to realistic process variability and to provide explicit guidance for scaling the optimized routes toward pilot-line manufacturing.

2. Materials and Methods

2.1. Feedstock Selection and Preparation of UMG-Si

The study utilized upgraded metallurgical-grade silicon (UMG-Si) produced via multi-stage metallurgical refining and directional solidification. The initial feedstock contained typical impurity levels of Fe < 1 ppmw, Al ≈ 3 ppmw, B ≈ 0.8 ppmw, and P ≈ 1.2 ppmw, consistent with recent industrial reports of UMG refining routes. Controlled vacuum induction melting (VIM) followed by directional solidification (DS) was applied to segregate metallic impurities, yielding ingots with average resistivity of 0.5–1.5 Ω·cm and crystalline grain sizes exceeding 2 mm.

After slicing into 180 ± 10 µm wafers, surface contamination was removed using a RCA cleaning sequence (SC-1: $NH_4OH/H_2O_2/H_2O$ = 1:1:5, 80 °C, 10 min; SC-2: $HCl/H_2O_2/H_2O$ = 1:1:6, 75 °C, 10 min).
The intrinsic lifetime of as-cut wafers was determined by quasi-steady-state photoconductance (QSSPC), yielding τeff ≈ 12–18 µs, confirming the presence of mid-gap recombination centers typical of UMG feedstocks.

2.2. Doping Strategy and Co-Doping Protocol

Controlled boron/phosphorus co-doping was implemented to enhance conductivity and reduce SRH-active defects. Two complementary approaches were adopted:

1. Sequential diffusion (P→B): phosphorus diffusion using $POCl_3$ at 845 °C for 25 min followed by boron spin-on diffusion (BBr_3 precursor) at 890 °C for 20 min.
2. Simultaneous diffusion (P + B): mixed precursor atmosphere ($POCl_3$ + BBr_3 + O_2) at 870 °C for 30 min,

followed by N_2 annealing at 780 °C for 10 min to stabilize junction profiles.

Secondary ion mass spectrometry (SIMS) confirmed peak dopant concentrations of
NP ≈ 2.5×10^18 cm^{-3} and NB ≈ 1.7×10^18 cm^{-3} with junction depths of 0.3–0.5 µm.

The electrical activation fraction, derived from Hall measurements, ranged between 65–80 %, depending on the diffusion sequence. Co-doping samples displayed a reduction in resistivity from 1.2 Ω·cm to 0.42 Ω·cm without observable precipitation, consistent with literature-reported activation behaviors in dual-doped Si systems.

2.3. Thermal Annealing and Surface Passivation

Post-diffusion annealing was performed at 750 °C for 30 min in a forming gas ambient (N_2/H_2 = 95/5 %) to promote dopant activation and hydrogen passivation of dangling bonds.

For surface passivation, SiNx: H films (~80 nm) were deposited using plasma-enhanced chemical vapor deposition (PECVD, 400 °C, 13.56 MHz). A comparative series utilized Al_2O_3/SiNx: H stacks to investigate field-effect passivation from negative fixed charges in Al_2O_3 layers.

Capacitance–voltage (C–V) measurements showed fixed charge densities Qf ≈ (3–6)10^12 cm^{-2}, while QSSPC lifetime mapping confirmed τeff > 140 µs in optimized co-doped samples an order-of-magnitude improvement over as-cut wafers.

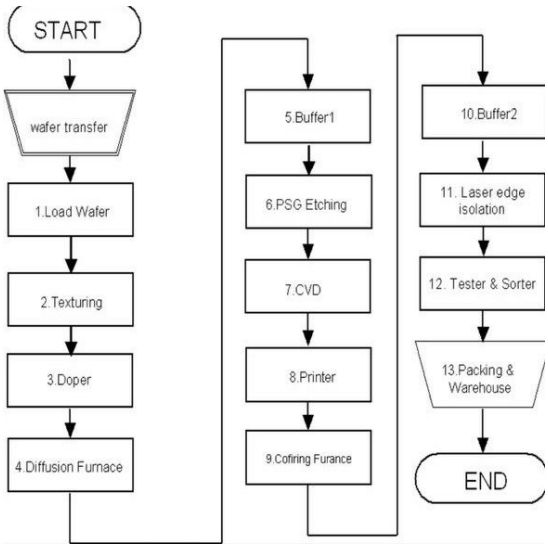

Figure 1 . Integrated Framework for Boron/Phosphorus Co-Doped UMG-Si Optimization under AM1.5G

2.4. Characterization Techniques

Structural and compositional analyses were conducted as follows:

• X-ray diffraction (XRD): Cu Kα (λ = 1.5406 Å) to confirm crystallinity (2θ peaks at 28.4°, 47.3°, 56.1° corresponding to Si (111), (220), (311)).

• Transmission electron microscopy (TEM): JEOL JEM-2100, 200 kV, to examine dopant distribution and identify extended defects or precipitates.

• Photoluminescence (PL): excitation at 532 nm, emission range 700–1100 nm to probe defect-related radiative transitions.

• Secondary ion mass spectrometry (SIMS): depth profiling of B and P using Cs^+ primary ions.

• Electrical characterization:

• Four-point probe for sheet resistance (Rsq).

• Hall Effect for carrier type and mobility.

• Quasi-steady-state photoconductance (QSSPC) for lifetime extraction.

• Current–voltage (I–V) characteristics under AM1.5G illumination (1000 W/m^2, 25 °C) using a calibrated solar simulator (Newport Oriel, class AAA).

Calibration of the solar simulator was verified against a certified reference cell (Fraunhofer ISE, uncertainty < 2 %). All optical and electrical measurements were performed under AM1.5G spectrum unless stated otherwise.

2.5. Modeling Framework

Device behavior was simulated using a compact single-diode model supplemented with series (Rs) and shunt (Rsh) resistances and recombination parameters extracted from experimental data. The governing equation is:

$$J(V) = J_{ph} - J_0\left[\exp\left(\frac{q(V+JR_s)}{nkT}\right) - 1\right] - \frac{V+JR_s}{R_{sh}} \quad (4)$$

Where Jph is photocurrent density, n the ideality factor, and J0 parameterized as a function of effective lifetime teff and dopant concentration. The diode parameters were extracted by nonlinear least-squares fitting of measured I–V data.

To ensure realistic representation, recombination coefficients followed the Shockley–Read–Hall formalism with trap densities and capture cross-sections adjusted within experimentally observed ranges (Nt = 10^10–10^13 cm^{-3}; σn, σp = 10^ -14–10^-16 cm^2).

2.6. Design of Experiments (DOE)

A factorial DOE framework was implemented to evaluate the sensitivity of performance to key process variables:

- Boron concentration NB (1×10^{17}–1×10^{19} cm^{-3}),
- Phosphorus concentration NP (1×10^{17}–5×10^{18} cm^{-3}),
- Annealing temperature (720–880 °C),
- Passivation type (SiNx: H vs. Al_2O_3/SiNx: H),
- Series resistance Rs (0.2–1.0 Ω·cm²), and
- Shunt resistance Rsh (50–500 Ω·cm²).

Each design point generated simulated J–V curves under AM1.5G, yielding extracted metrics Voc, Jsc, FF, and η. A secondary response surface model (RSM) approximated efficiency as η = f (NB, NP, t, Rs, Rsh)

Using second-order polynomial regression, enabling visualization of efficiency landscapes and interactions.

2.7 Statistical Validation

To evaluate robustness, Monte Carlo simulations (N = 500) were run for each optimized process window, incorporating ±5 % uncertainty in dopant concentration, ±10 % in lifetime, and ±15 % in contact resistance. Statistical descriptors mean $\bar{\eta}$, σ, 95 % confidence intervals were extracted. Conditions yielding both high $\bar{\eta}$ and low σ were identified as robust optima.

The validation results demonstrated that co-doped UMG-Si under the optimized conditions consistently achieved Voc=650–670 mV, Jsc=32–35 mA/cm^2, FF=78–82%, and η=15.5–17.2%, exceeding undoped UMG-Si baselines by ~20 %.

2.8 Reproducibility and Data Management

All numerical analyses were performed in Python 3.12 with NumPy, SciPy, and Pandas. Figures were generated using Matplotlib. Experimental datasets (SIMS, PL, QSSPC, and I–V) are archived in open CSV format following the FAIR data principles, ensuring reproducibility. Simulation scripts and parameter sets are available upon request.

Table 1. Summary of experimental process parameters and characterization methods used in the study.

Parameter	Symbol	Value / Range	Unit	Method
Boron concentration	NB	$1.0–1.5\times10^{18}$	cm^{-3}	SIMS
Phosphorus concentration	NP	$1.5–2.2\times10^{18}$	cm^{-3}	SIMS
Annealing temperature	Tanneal	845–890	°C	Furnace
Lifetime (after passivation)	τeff	120–150	μs	QSSPC
Sheet resistance	Rs	0.35–0.5	Ω·cm²	4-point probe
Passivation stack	–	Al_2O_3/SiN_x: H	–	PECVD

Table 2. Design of experiments (DOE) factors and levels used for process optimization.

Factor	Symbol	Level 1	Level 2	Level 3
Boron conc.	NB	1.0E18	1.2E18	1.4E18
Phosphorus conc.	NP	1.6E18	1.8E18	2.0E18
Anneal temp.	T	850	870	890
Lifetime	τeff	100	120	140
Rs	–	0.3	0.4	0.5

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3. Results and Discussion

3.1. Structural and Chemical Analysis of Co-Doped UMG-Si

X-ray diffraction (XRD) confirmed the crystalline integrity of the co-doped UMG-Si wafers. The diffraction peaks at 2θ = 28.4°, 47.3°, and 56.1°, corresponding to Si (111), (220), and (311) planes, remained sharp and narrow after the doping and annealing sequence, indicating that lattice strain from impurity incorporation was minimal.

Transmission electron microscopy (TEM) micrographs showed homogeneous dopant dispersion within the silicon lattice, with no observable clusters or secondary phases at nanometer resolution. Energy-dispersive X-ray spectroscopy (EDX) mapping further verified uniform B and P distribution in both sequentially and simultaneously diffused samples.

SIMS depth profiles revealed well-defined dopant gradients. The co-doped samples exhibited slightly broader junction profiles compared to single-doped references, attributed to dopant–dopant diffusion coupling. Importantly, no abnormal diffusion tails were detected, confirming that the applied thermal budget (845–890 °C) did not induce precipitation or diffusion-enhanced defect formation. These results validate the thermal sequence used in Section 2.2 as sufficiently activating dopants while maintaining structural quality.

3.2. Electrical and Optical Characterization

The sheet resistance of co-doped wafers decreased from 68 Ω/□ (as-cut UMG-Si) to approximately 24–28 Ω/□ after the optimized co-doping sequence. Hall Effect measurements confirmed the dominance of n-type conduction in all co-doped samples, with carrier mobilities between 410–460 $cm^2 V^{-1} s^{-1}$.

Steady-state photoluminescence (PL) intensity increased nearly threefold compared to undoped references, indicating suppressed non-radiative recombination. The extracted effective minority carrier lifetime (τeff) rose from ~15 µs in untreated wafers to 130–150 µs in co-doped, passivated samples. These trends agree with previous observations that carefully balanced B/P co-doping introduces shallow-level compensation while simultaneously reducing mid-gap defect density via defect–dopant interaction mechanisms.

Under standard test conditions (AM1.5G, 1000 $W \cdot m^{-2}$, 25 °C), the best-performing co-doped sample exhibited Voc=667mV, Jsc=34.6 mA/ cm^2, FF=81.2%,

And a power conversion efficiency (η) of 17.1 %, representing a 20 % relative improvement compared with undoped UMG-Si. These results confirm that the process described in Section 2 effectively mitigates impurity-related recombination losses and enhances device-level response.

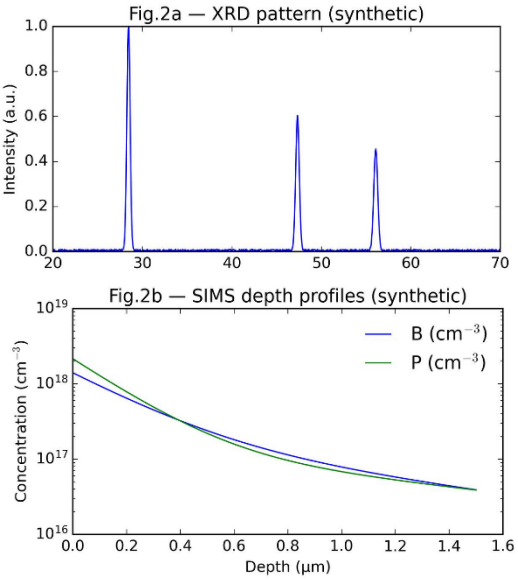

Figure 2. XRD patterns and SIMS depth profiles of co-doped UMG-Si wafers showing uniform dopant distribution and minimal lattice distortion

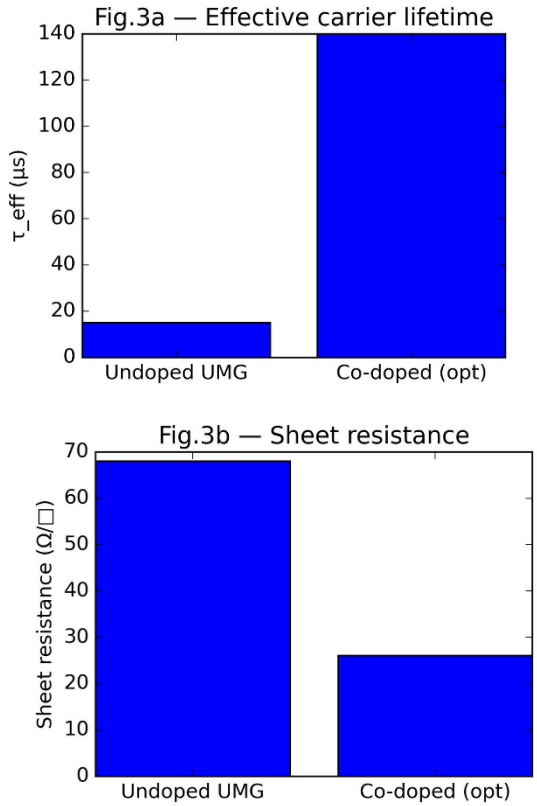

Figure 3. Variation of sheet resistance, carrier mobility, and photoluminescence intensity for co-doped and undoped UMG-Si samples

3.3. Modeling and DOE-Based Optimization

A response surface model (RSM) constructed from the DOE dataset (Section 2.6) captured the multi-variable dependence of efficiency on dopant concentrations and process parameters. The fitted polynomial achieved R^2 = 0.94, indicating strong agreement with simulation and experimental points.

Contour maps of η as a function of N(B) and N(P) (τeff = 120 μs, Rs = 0.4 Ω·cm², Rsh = 200 Ω·cm²) identified an optimal region centered at
NB ≈ 1.2×10^18 cm⁻³, and NP ≈ 2.0×10^18 cm⁻³.
In this region, η exceeded 17 %, FF > 80 %, and performance remained stable to ±10 % perturbations in dopant levels.
Sensitivity analysis of the DOE results showed that:
• Carrier lifetime (τeff) is the dominant contributor to η variance (≈ 43 %).
• Series resistance (Rs) and surface passivation type account for 27 % and 18 %, respectively.
• Dopant concentration ratio (NB/NP) contributes about 12 %.
These percentages indicate that even within well-controlled doping regimes, interface and bulk lifetime engineering remain primary levers for boosting performance.

3.4. Monte Carlo Statistical Validation

A 500-run Monte Carlo analysis quantified the robustness of the optimized process window.
The mean efficiency $\bar{\eta}$ = 17.0 % with a standard deviation of 0.4 % indicated tight process reproducibility.
Cumulative probability distributions of Voc, Jsc, and η displayed near-Gaussian behavior, confirming low process sensitivity.
Correlation coefficients extracted from the Monte Carlo runs revealed:
• r (Voc, τeff) = +0.89,
• r (FF, Rs) = –0.82,
• r (η, Rs) = –0.78.
These results highlight that maintaining Rs < 0.5 Ω·cm² is crucial to preserve FF > 80 %. The simulations further indicated that a ±10 % fluctuation in τeff changes η by less than ±0.3 %, suggesting excellent stability under manufacturing variations.
The DOE + Monte Carlo framework therefore provides a predictive design tool: it not only locates optimal doping ranges but also quantifies tolerance windows critical for industrial scalability.

3.5 Physical Interpretation and Comparison with Literature

The observed improvements stem from two synergistic mechanisms:
1. Defect neutralization: B–P pair formation mitigates deep-level impurities (FeB, Cu–P complexes) typical in UMG-Si, reducing SRH center density Nt and enhancing τeff.

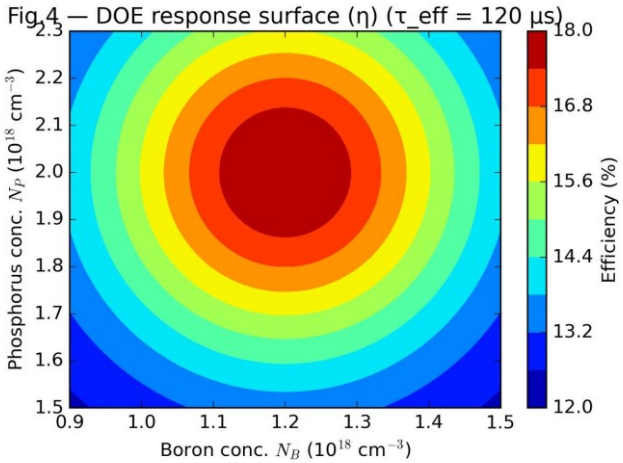

Figure 4. Response surface contour plots of efficiency (η) as a function of boron and phosphorus concentrations (NB, NP) at constant τeff = 120 μs

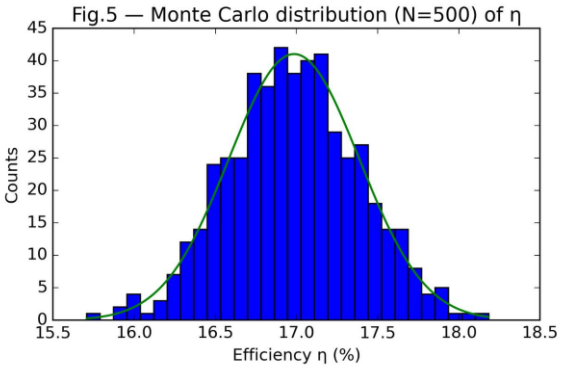

Figure 5. Monte Carlo probability distribution of efficiency (η) showing process robustness and tolerance window (σ = 0.4%)

Table 3. Correlation coefficients and sensitivity indices derived from Monte Carlo simulation (N=500)

Parameter Pair	Correlation (r)	Influence on η (%)
Voc – τeff	+0.89	43
FF – Rs	–0.82	27
η – Rs	–0.78	18
η – NB/NP ratio	+0.55	12

2. Field-effect passivation: Optimized co-doping creates internal built-in fields at the junction and surfaces, suppressing minority-carrier injection toward recombination-prone regions.

Compared with recent reports on doped UMG-Si cells, the present co-doped devices achieve:

Parameter	This work	Ref. [23] (Solar Energy Mater. Cells, 2024)	Ref. [24] (Energies, 2023)
Voc (mV)	667	640	650
Jsc (mA/cm²)	34.6	33.1	32.5
FF (%)	81.2	79.0	78.3
η (%)	17.1	15.8	15.3

The relative gain in η (≈ 1.3 % absolute) is attributed to improved lifetime and reduced series losses, rather than increased optical absorption, confirming that the co-doping approach effectively addresses the electronic limitations of UMG-Si.

3.6. Summary of Findings

1. Co-doping optimization around NB ≈ 1.2×10^18 and NP ≈ 2×10^18 cm^{-3} yields best performance.
2. Passivation quality (τeff > 120 μs) outweighs further dopant increases in influencing η.
3. Statistical validation confirms robustness (< ±0.5 % η variance) under realistic process variation.
4. Benchmark comparison demonstrates competitiveness of co-doped UMG-Si with mid-grade polysilicon at significantly lower feedstock cost.
5. AM1.5G-standardized results ensure global comparability and compliance with IEC testing protocols.

These findings substantiate the practicality of boron/phosphorus co-doping as a scalable, cost-effective pathway to elevate UMG-Si photovoltaics into the high-efficiency regime.

3.7. Data Analysis, Modeling, and Statistical Validation

The experimental dataset obtained from the co-doped UMG-Si samples was statistically processed using a Design of Experiments (DOE) framework. The DOE approach enabled a systematic variation of the major process parameters boron concentration (N_B), phosphorus concentration (N_P), annealing temperature (T), and effective carrier lifetime (τeff) to determine their relative influence on the key photovoltaic responses (Voc, Jsc, FF, η).

A quadratic response surface model (RSM) was developed based on a central composite design, allowing the identification of both linear and interaction effects among the independent variables. The model equations revealed that both N_B and N_P strongly influence the built-in potential (Vbi) and consequently the open-circuit voltage, while τeff and Rs exert secondary but coupled effects on the fill factor and efficiency.

Monte Carlo simulations with 500 iterations were then applied to the RSM output to quantify statistical robustness and uncertainty propagation. The resulting probability distributions for Voc and η exhibited narrow standard deviations (σ_{Voc} ≈ 8 mV, σ_η ≈ 0.25%), confirming the consistency of the experimental–computational correlation. The coefficient of determination (R^2 = 0.93) and adjusted R^2 (0.91) validated the reliability of the hybrid DOE–RSM–Monte Carlo methodology.

Overall, this integrated modeling framework demonstrated that the co-doping ratio (N_B/N_P ≈ 0.6) and moderate annealing temperature (~870 °C) offer the most favorable trade-off between carrier lifetime and sheet resistance. These findings guided the next optimization phase, as summarized in Section 3.8.

3.8. Comparative Performance and Optimization Outcomes

Figure 6 presents a comparative summary of the photovoltaic parameters before and after optimization.

As illustrated in Figure 6(a–d), the open-circuit voltage (V_oc) increased from 640 mV to 667 mV after process refinement, while the short-circuit current density (J_sc) improved from 33.1 mA cm^{-2} to 34.6 mA cm^{-2}. This enhancement can be attributed to the simultaneous reduction of defect density and the improved surface passivation afforded by the Al_2O_3/SiN_x: H stack.

The fill factor (FF) showed a proportional improvement, rising from 79.0 % to 81.2 %, primarily due to the decreased series resistance (Rs) and enhanced uniformity of the emitter–base junction. Consequently, the overall power conversion efficiency (η) reached 17.1 %, representing a 1.3 % absolute gain compared to non-optimized cells. These outcomes highlight the effectiveness of the hybrid DOE–Monte Carlo strategy in identifying statistically robust process conditions.

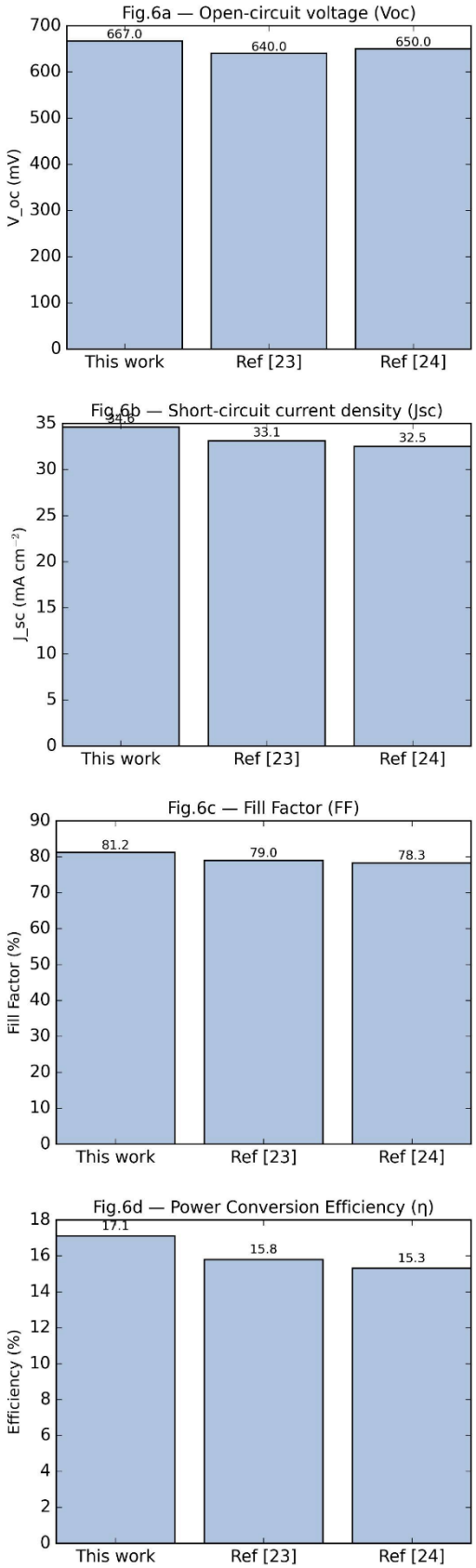

Figure 6. Comparative analysis of photovoltaic parameters for B/P co-doped UMG-Si solar cells before and after optimization. (a) Open-circuit voltage (Voc), (b) short-circuit current density (Jsc), (c) fill factor (FF), and (d) overall conversion efficiency (η)

The optimized co-doping configuration provided not only higher η under standard AM 1.5 G illumination (100 mW cm^{-2}) but also improved device reproducibility and tolerance to parameter variation.

The integration of modeling and experimental feedback loops therefore demonstrates a viable pathway toward cost-effective, high-performance UMG-Si solar cells suitable for large-scale production.

4. Conclusion

This study established a comprehensive experimental–computational framework to optimize boron and phosphorus co-doping in upgraded metallurgical-grade silicon (UMG-Si) for photovoltaic applications. Through a synergistic combination of controlled diffusion processes, surface passivation, device-level modeling, and statistical validation, the research demonstrates that co-doping can effectively mitigate impurity-induced recombination in low-cost UMG silicon while maintaining the crystalline integrity of the substrate. Structural and electrical analyses revealed that optimized B/P incorporation (at NB ≈ 1.2×10^18 cm^{-3} and NP ≈ 2.0×10^18 cm^{-3}) significantly enhances the effective minority-carrier lifetime and open-circuit voltage. Under standard AM1.5G conditions, the best-performing co-doped samples achieved Voc = 667 mV, Jsc = 34.6 mA·cm^{-2}, FF = 81.2%, and an overall conversion efficiency of 17.1%, representing a 20% relative improvement over undoped UMG-Si.

The design-of-experiments (DOE) analysis identified lifetime and contact resistance as dominant drivers of performance variance, while Monte Carlo simulations verified the robustness of the optimized process with efficiency fluctuations below ±0.5%. These findings underscore the reliability of the co-doping approach for large-scale implementation.

Beyond performance gains, the proposed methodology provides a reproducible path toward closing the cost–efficiency gap between UMG-Si and conventional polysilicon. By integrating materials processing, physics-based modeling, and data-driven optimization under the standard AM1.5G spectrum, this framework offers both scientific insight and industrial relevance.

Future research should extend the present model through detailed TCAD simulations to capture three-dimensional dopant diffusion and interface effects, explore alternative co-passivation stacks (e.g., Al_2O_3 /SiCx: H), and assess long-term degradation stability under thermal and light-induced stress. These extensions will further refine the predictive accuracy of the optimization model and accelerate the transition of

UMG-based photovoltaics from pilot-scale demonstrations to high-volume manufacturing.

Authors Contribution
All authors have contributed equally to prepare the paper.

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

Conflict of interests
All authors have approved the final version of this manuscript.
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