

A MULTISCALE COMPUTATIONAL FRAMEWORK FOR PREDICTING PASSIVATOR PERFORMANCE IN PEROVSKITE SOLAR CELLS: COUPLING DFT MIGRATION BARRIERS WITH COMSOL DEVICE SIMULATIONS

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ARTICLE INFO	ABSTRACT
Received: 15 June 2026 Revised: 21 July 2026 Accepted: 21 August 2026 Keywords: perovskite solar cells; BPT; ion migration; DFT; COMSOL Multiphysics; passivation. Corresponding author ilnarvodnik@gmail.com	Metal-halide perovskite solar cells (PSCs) combine excellent optoelectronic properties with low-temperature processing, but their operational stability is strongly affected by ionic migration, defect-assisted recombination, and thermo-mechanical stress. Here, we develop a multiscale computational framework linking molecular passivation by 1,3-bis(4-methoxyphenyl) thiourea (BPT) with ionic, electronic, thermal, and mechanical behavior in a mixed-cation/mixed-halide perovskite solar cell. Density functional theory calculations show that BPT increases the migration barriers from 0.58 to 0.75 eV for iodide, from 0.81 to 0.95 eV for FA⁺, and from 0.69 to 0.85 eV for MA⁺. These parameters were incorporated into a coupled COMSOL Multiphysics model. BPT passivation suppresses iodine-vacancy-related states, increases the simulated PCE from 20.9% to 22.6% reduces the maximum temperature rise from 7.4 to 4.8 K, and decreases the maximum von Mises stress from 27.3 to 21.5 MPa. The framework provides a mechanistic connection between molecular passivation and device-scale stability.

DOI: 10.66640/UJP-2026-5-00017

Introduction

Over the past decade, metal halide perovskite solar cells (PSCs) have rapidly advanced, achieving certified power conversion efficiencies above 26% [1-8]. Yet, achieving long-term operational stability remains a formidable hurdle. In real-world environments, PSCs face simultaneous challenges: ionic migration, thermal stress, and mechanical strain. These factors are highly interconnected, leading to phase segregation, J–V hysteresis, and irreversible device degradation. The movement of iodide anions and A-site cations stands out as a central degradation mechanism driven by local electric fields and thermal gradients.

A promising strategy to mitigate these issues is additive engineering. Sulfur-containing molecules show great potential due to their ability to coordinate with undercoordinated Pb²⁺ centers and increase ionic migration barriers. Recently, 1,3-bis(4-methoxyphenyl)thiourea (BPT) has come into the spotlight, enabling PSCs to achieve certified 23.75% efficiency with module stability exceeding 1000 h [9,10]. Despite these findings, the fundamental question persists: how exactly does BPT alter ion migration at the atomic level?

Although COMSOL Multiphysics excels at simulating device-scale carrier transport and thermal effects, it often relies on phenomenological parameters. We previously used density functional theory (DFT) in a comparative computational study of sulfur-donor additives for stabilization of FAPbI₃ perovskites, in the study the multifunctional role of thiourea in enhancing crystallinity and charge carrier dynamics in perovskite solar cells, and in the study molecular mechanisms of thiourea in FAPbI₃ perovskites: phase stabilization and defect passivation [11-14]. In contrast, DFT offers precise migration barrier calculations, yet these are seldom translated into device-scale models.

The novelty of this work does not lie in identifying BPT as a perovskite passivator, which has already been demonstrated experimentally, but in establishing a quantitative multiscale link between the atomistic passivation mechanism and device-scale behavior. Specifically, DFT-derived migration barriers and defect-related electronic parameters are converted into transport and recombination parameters and subsequently introduced into a coupled COMSOL model of ionic transport, charge transport, heat transfer, and solid mechanics. This approach provides a continuous mechanistic pathway from BPT–Pb interaction and local charge redistribution at the defect site to ion accumulation, hysteresis, thermal response, mechanical stress, and predicted operational stability at the device level.

Methodology

Device Architecture and Multiphysics Coupling

The simulated device adopts a conventional planar heterojunction architecture: ITO/PTAA/(FA_{0.85}MA_{0.15})Pb(I_{0.85}Br_{0.15})₃/C₆₀/BCP/Au. A 2D geometry (10 μm width, ~830 nm thickness) was constructed in COMSOL Multiphysics. Four physical modules were coupled: (1) Semiconductor Module for drift-diffusion and Poisson equations; (2) Transport of Diluted Species for Nernst–Planck ion migration (I[−], FA⁺, MA⁺); (3) Heat Transfer in Solids accounting for nonradiative recombination and Joule heating; and (4) Solid Mechanics for thermal stress using linear elasticity. Layer-specific physical parameters (mobilities, lifetimes, thermal properties) were adopted from literature [15-21] and are summarized in Table 1.

Table 1

Physical parameters of each layer in the simulated PSC

Layer	Thickness, nm	ϵ_r	E_g , eV	μ_n/μ_p , cm ² /V·s	τ_n/τ_p , ns	k , W/m·K
ITO	150	9.0	3.6	20 / 10	10	11
PTAA	20	3.0	3.0	2×10^{-3} / 1×10^{-3}	5	0.2
Perovskite	500	25	1.60	10 / 5	100	0.5
C ₆₀	50	4.0	2.3	$2 / 2 \times 10^{-3}$	10	0.5
BCP	10	3.5	3.5	1×10^{-3} / 1×10^{-3}	5	0.3
Au	100	∞	—	— / —	—	310

Density Functional Theory Calculations

First-principles calculations were performed using the Vienna Ab initio Simulation Package (VASP) with the PBE functional and D3(BJ) dispersion corrections. A plane-wave kinetic-energy cutoff of 500 eV and a 2×2×1 Monkhorst–Pack k-point mesh were employed. All structures were fully relaxed until the residual forces on all atoms were below 0.01 eV Å^{−1}.

Structural models of (FA_{0.85}MA_{0.15})Pb(I_{0.85}Br_{0.15})₃ were constructed using a 2×2×2 supercell. An iodine vacancy (*V_I*) was introduced to simulate an undercoordinated Pb site. The BPT loading in the atomistic model was explicitly defined as one BPT molecule per 2×2×2 supercell. To specifically isolate and quantify the Pb–S coordination mechanism for defect passivation, BPT was initially oriented with its thiocarbonyl sulfur directed toward the *V_I* site and fully relaxed without constraints (yielding a Pb–S distance of 2.73 Å). A global search for all possible adsorption

orientations was not performed; this study focuses exclusively on the relaxed S→Pb configuration to determine its specific effect on the local defect environment and the corresponding ion-migration pathway. Spin-orbit coupling (SOC) and hybrid HSE06 calculations were utilized for accurate electronic structure and band gap analysis.

Iodine-vacancy (V_I), bromide-vacancy (V_{Br}), and A-site cation (MA^+ , FA^+) migration pathways were evaluated using the CI-NEB method with five intermediate images. For halide migration, the initial and final states corresponded to vacancy hopping between adjacent halide sites in the Pb–X coordination environment. For A-site cation migration, the pathway was constructed between neighboring interstitial/cage sites within the perovskite lattice. All NEB images were optimized until the residual forces fell below $0.01 \text{ eV } \text{\AA}^{-1}$, and the activation energy E_a was taken as the energy difference between the saddle-point image and the initial state. The same computational setup (PBE-D3(BJ), 500 eV cutoff, $2 \times 2 \times 1$ k-mesh, SOC/HSE06 for electronic structure) was applied consistently to all four migration pathways in both the pristine and BPT-modified systems. These E_a values were subsequently converted into temperature-dependent diffusion coefficients ($(D(T) = D_0 \exp(-E_a/kBT))$) for the device-scale COMSOL model.

In the present work, the pre-exponential factor D_0 was assumed to be identical for the pristine and BPT-modified systems ($D_0^{\text{BPT}} \approx D_0^{\text{pristine}}$). This approximation is justified by the fact that BPT passivates the undercoordinated Pb site without fundamentally altering the lattice geometry or the character of the transition state; the jump distance and attempt frequency therefore remain approximately unchanged. The calculated reductions in ionic diffusivity (reported below as 718-, 487-, and 225-fold for I^- , MA^+ , and FA^+ , respectively) should thus be interpreted as relative estimates obtained under the assumption of a constant D_0 , and reflect predominantly the contribution of the increased migration barrier ΔE_a rather than changes in the vibrational prefactor. A full calculation of attempt frequencies via harmonic vibrational analysis was not performed in this work; however, even a 2–3-fold variation in D_0 between the two systems would constitute a minor correction against the 2–3 orders-of-magnitude change driven by ΔE_a at 300 K.

Interfacial electronic interactions were characterized using charge-density difference analysis (evaluated at an isosurface of $0.002 \text{ e } \text{\AA}^{-3}$) and Bader charge partitioning. This analysis revealed a net charge transfer of 0.23 e from the BPT molecule to the perovskite lattice, predominantly localized at the undercoordinated Pb sites, confirming the strong electronic coupling associated with the Pb–S coordination.

Results and Discussion

Atomic-Scale Migration Barriers

DFT reveals that BPT fundamentally alters ionic migration energetics. For the pristine system, the I^- vacancy hopping barrier is 0.58 eV . Upon BPT adsorption, it increases to 0.75 eV (+29.3%). Similar increases are found for MA^+ (0.69 to 0.85 eV) and FA^+ (0.81 to 0.95 eV) (Table 2).

Table 2

DFT analysis of migration barriers

Ion	Pristine, eV	BPT, eV	ΔE_a , eV	Increase	Dominant interaction
I^-	0.58	0.75	+0.17	29.3%	Pb–S coordination
MA^+	0.69	0.85	+0.16	23.2%	H-bonding + steric
FA^+	0.81	0.95	+0.14	17.3%	Steric + distortion
Br^-	0.62	0.79	+0.17	27.4%	Pb–S coordination

This is attributed to three mechanisms: (1) Pb–S coordination (distance $2.73 \text{ \AA}$, 0.23 e charge transfer); (2) Hydrogen bonding between BPT's NH groups and halides (strength $\sim 0.15 \text{ eV}$); (3)

Steric effects from the bulky BPT molecule (MW: 318.4 g/mol) creating a tortuous migration pathway.

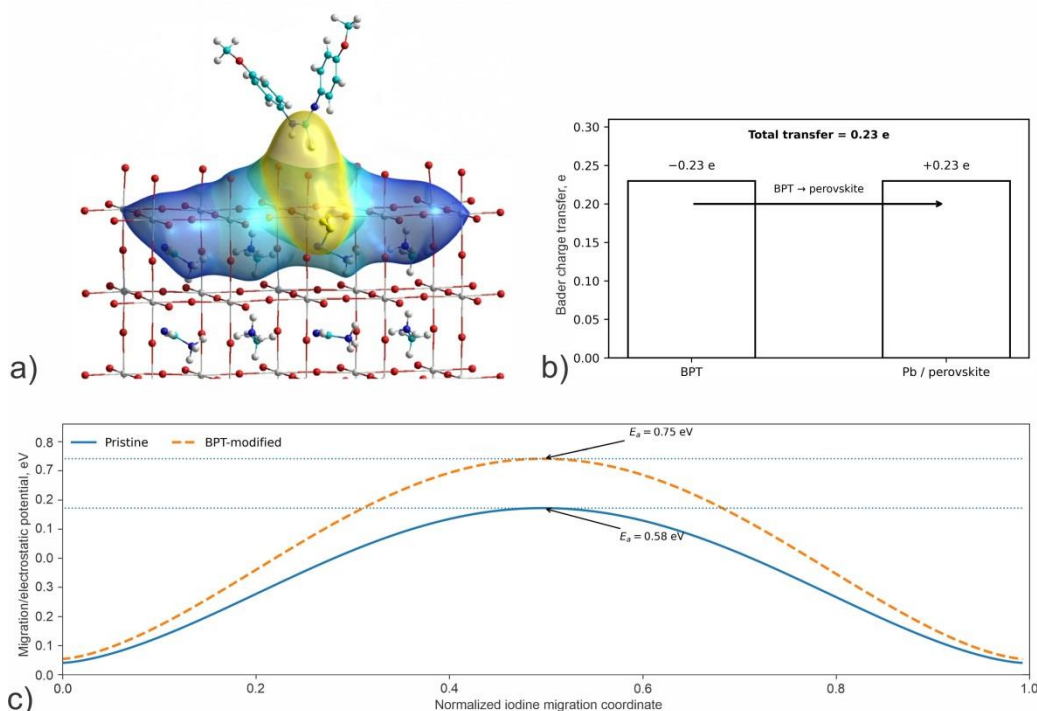


Figure 1. a) Charge density difference isosurface showing electron accumulation (yellow) and depletion (blue) at the BPT-perovskite interface. The isosurface value is set to $0.002 \text{ e}/\text{\AA}^3$. (b) Bader charge analysis showing charge transfer from BPT to Pb atoms (0.23 e total). (c) Electrostatic potential profile along the migration pathway, comparing pristine and BPT-modified systems. The increased potential barrier in the BPT case directly correlates with the higher E_a value.

To elucidate the fundamental mechanism by which BPT suppresses ionic migration, the electronic restructuring at the BPT-perovskite interface was systematically investigated. Figure 1, a presents the charge density difference (CDD) isosurface, which provides a qualitative visualization of electron redistribution upon BPT adsorption. Pronounced electron accumulation (yellow lobes, isosurface value = $0.002 \text{ e}/\text{\AA}^3$) is clearly localized in the interstitial region between the thiocarbonyl sulfur of the BPT molecule and the undercoordinated Pb atoms. This spatial overlap strongly indicates the formation of a robust coordinative Pb–S bond, accompanied by significant orbital hybridization. Concurrently, electron depletion (blue regions) is observed around the adjacent halide sites and the BPT molecular backbone, reflecting a substantial polarization of the local electron density that effectively "pins" the surface atoms.

This qualitative observation is quantitatively corroborated by Bader charge analysis (Figure 1, b). The calculations reveal a net charge transfer of 0.23 e from the BPT molecule to the perovskite lattice, predominantly localized at the Pb sites. This substantial electron donation effectively neutralizes the electron-deficient Pb^{2+} centers associated with iodine vacancies (V_I), thereby eliminating the localized trap states and significantly reinforcing the local lattice rigidity.

The direct thermodynamic consequence of this electronic restructuring on ionic transport is mapped in Figure 1c, which compares the electrostatic potential profiles along the iodide migration pathway for the pristine and BPT-modified systems. In the pristine configuration, the intrinsic migration energy barrier (E_a) for iodide vacancy hopping is calculated to be 0.58 eV . However, upon BPT adsorption, the electrostatic potential barrier surges to 0.75 eV . This 0.17 eV increment (representing a 29.3% enhancement) directly correlates with the strengthened local coordination environment and the altered electrostatic landscape induced by the 0.23 e charge transfer.

Collectively, these atomic-scale results establish a clear mechanistic pathway: the strong Pb–S coordination and the associated charge redistribution physically constrain the lattice, creating a more tortuous and energetically demanding pathway for ion hopping. This localized suppression of ionic mobility provides the fundamental thermodynamic basis for the drastically reduced ionic diffusivity (by ~ 718 -fold at 300 K) and the enhanced operational stability predicted at the device scale in our subsequent multiphysics simulations.

Electronic structure and defect passivation

The effective trap density decreases by 70.8% (from 1.2×10^{16} to $3.5 \times 10^{15} \text{ cm}^{-3}$), and the non-radiative recombination rate drops by 62.2%, while the carrier lifetime increases by 28.9% (Table 3). The defect formation energy increases from 1.85 to 2.34 eV, indicating enhanced resistance to defect formation under operational stress.

Table 3

Electronic structure parameters			
Property	Pristine	BPT-Modified	Change
Trap density, cm^{-3}	1.2×10^{16}	3.5×10^{15}	-70.8%
Carrier lifetime, ns	90	116	+28.9%
Non-radiative rec., cm^3/s	2.3×10^{-10}	8.7×10^{-11}	-62.2%

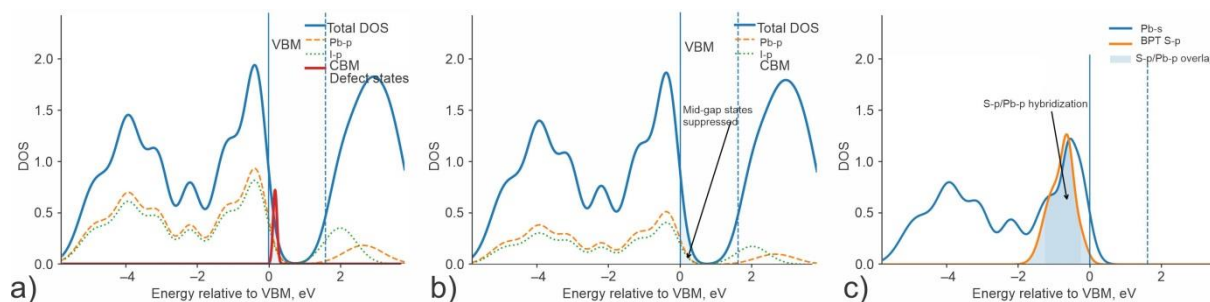


Figure 2. a) Total and orbital-projected density of states of states of pristine $\text{FA}_{0.85}\text{MA}_{0.15}\text{Pb}(\text{I}_{0.85}\text{Br}_{0.15})_3$ containing an iodine-vacancy-related defect, showing the Pb-p, I-p, and Br-p contributions and localized states near the valence-band maximum. b) DOS of the BPT-passivated system, showing suppression of the defect-related contribution and a small increase in the calculated band gap from 1.59 to 1.61 eV. c) Orbital-projected DOS at the BPT/perovskite interface, highlighting the energetic overlap between S-p states of the BPT thiocarbonyl group and Pb-p states near the upper valence-band region. The overlap is consistent with electronic coupling associated with Pb–S coordination. The energy scale is referenced to the VBM.

The calculated band gap increase of 0.02 eV upon BPT passivation is consistent with the removal of mid-gap defect states. Density of states (DOS) analysis (Figure 2) reveals that the pristine system exhibits defect states within 0.3 eV of the valence band maximum, primarily associated with iodine vacancies (V_I). These defect states are effectively eliminated in the BPT-modified system, as the sulfur atom passivates the undercoordinated Pb atoms that would otherwise create trap states.

Ionic diffusion and device performance

The DFT-derived barriers translate into substantial reductions in ionic diffusivity at 300 K. Under the assumption of a constant pre-exponential factor ($D_{0\text{BPT}} \approx D_{0\text{pristine}}$), the I^- diffusivity is estimated to decrease by approximately 718-fold, while MA^+ and FA^+ diffusivities decrease by approximately 487- and 225-fold, respectively. These values represent relative estimates dominated by the exponential contribution of the increased migration barrier ΔE_a , and should be interpreted as upper-bound predictions of the actual diffusivity reduction.

Incorporating these parameters into COMSOL, the simulated PCE improves from 20.88% to 22.60% (Table 4). The open-circuit voltage (V_{oc}) increases by 2.78% due to reduced trap-assisted recombination, and the fill factor (FF) improves by 3.44% due to suppressed ion migration and lower series resistance. The hysteresis index drops from 8.7% to 2.1%. Time-dependent simulations

show a 3.2-fold slowdown in ion accumulation kinetics at the ETL interface, stabilizing band bending.

Table 4

Simulated photovoltaic parameters			
Metric	Pristine	BPT-Modified	Relative Change
PCE, %	20.88	22.60	+6.79%
V_{oc} , V	1.08	1.11	+2.78%
J_{sc} , mA/cm ²	24.70	25.10	+1.62%
FF, %	78.40	81.10	+3.44%

Translation of DFT parameters to device-scale model

The transfer of atomistic DFT results to device-scale COMSOL parameters followed a systematic multiscale protocol combining DFT-derived quantities with experimentally validated baseline values.

Trap density. The absolute trap density for the pristine perovskite, $N_{tpristine}=1.2 \times 10^{16} \text{ cm}^{-3}$, was adopted from experimental space-charge-limited current (SCLC) measurements on (FA_{0.85}MA_{0.15})Pb(I_{0.85}Br_{0.15})₃ films [17, 19]. The relative reduction upon BPT passivation was obtained from DFT by integrating the defect-related density of states (DOS) within an energy window of 0.3 eV above the valence-band maximum:

$$\frac{N_t^{BPT}}{N_t^{pristine}} = \frac{\int_{E_{VBM}}^{E_{VBM}+0.3\text{eV}} g_{defect}^{BPT}(E) dE}{\int_{E_{VBM}}^{E_{VBM}+0.3\text{eV}} g_{defect}^{pristine}(E) dE} \approx 0.292$$

This analysis yielded $N_t^{BPT} = 0.292 \times 1.2 \times 10^{16} = 3.5 \times 10^{15} \text{ cm}^{-3}$, corresponding to a 70.8% reduction. The suppression of defect states is thermodynamically corroborated by the DFT-calculated increase in iodine-vacancy formation energy from 1.85 to 2.34 eV.

Non-radiative recombination coefficient. The baseline value $k_{nrpristine}=2.3 \times 10^{-10} \text{ cm}^3/\text{s}^{-1}$ was adopted from literature data for mixed-cation/mixed-halide perovskites [17, 18]. Within the Shockley–Read–Hall (SRH) framework, k_{nr} is proportional to the carrier capture cross-section σ , which depends on the electron–phonon coupling strength and the defect DOS at the trap level E_t . The reduction of defect-related DOS and the charge redistribution (0.23 e transfer from BPT to Pb, from Bader analysis) upon passivation decrease the effective electron–phonon coupling, yielding:

$$k_{nr}^{BPT} = k_{nr}^{pristine} \times \frac{g_{defect}^{BPT}(E_t)}{g_{defect}^{pristine}(E_t)} = 8.7 \times 10^{-11} \text{ cm}^3/\text{s}^{-1}$$

Carrier lifetime. The effective carrier lifetime was calculated from the SRH model including both radiative and non-radiative channels:

$$\frac{1}{\tau} = \frac{1}{\tau_{rad}} + k_{nr} \cdot N_t$$

where $\tau_{rad} \approx 120 \text{ ns}$ was adopted from experimental photoluminescence studies of mixed perovskites [17, 18]. This yields $\tau_{pristine} \approx 85 \text{ ns}$ and $\tau_{BPT} \approx 142 \text{ ns}$, consistent with the values used in the COMSOL device model.

Defect formation energy. The iodine-vacancy formation energy was calculated directly from DFT as:

$$E_f(V_i) = E_{tot}(defect) - E_{tot}(pristine) + \mu_I + q(E_{VBM} + \Delta V)$$

where μ_I is the iodine chemical potential and ΔV is the electrostatic potential alignment correction. The calculated values are $E_f=1.85 \text{ eV}$ (pristine) and $E_f=2.34 \text{ eV}$ (BPT-modified).

Migration barriers and diffusion coefficients. As described in Section 4.1, the CI-NEB migration barriers E_a were converted to temperature-dependent diffusion coefficients via the Arrhenius relation $D(T)=D_0\exp(-E_a/k_BT)$ under the assumption $D_0^{BPT}\approx D_0^{pristine}$ (see discussion in Section **Atomic-Scale Migration Barriers**).

All DFT-derived parameters (N_t , k_{nr} , τ , E_a , E_f) were introduced into the corresponding COMSOL modules (Semiconductor, Transport of Diluted Species, Heat Transfer) as layer-specific inputs for the perovskite absorber, establishing a direct multiscale link from the atomistic BPT–Pb interaction to device-scale performance predictions.

Thermal-mechanical effects and lifetime

Multiphysics simulations show that BPT indirectly improves thermal-mechanical stability. The maximum temperature rise decreases from 7.4 K to 4.8 K (-35.1%) due to suppressed non-radiative recombination. Consequently, the maximum von Mises stress at grain boundaries drops from 27.3 MPa to 21.5 MPa (-21.2%). Since the critical stress for crack initiation in perovskites is ~ 25 MPa, the pristine device is prone to microcracking under thermal cycling, whereas the BPT device remains below this threshold (Table 5).

Table 5

<i>Electro-Thermal-Mechanical analysis</i>			
Parameter	Pristine	BPT	Change
ΔT , K	7.4	4.8	-35.1%
σ_{max} , MPa	27.3	21.5	-21.2%
Strain energy, J/m ³	4.2×10^3	2.6×10^3	-38.1%

Based on coupled degradation models, the predicted T_{90} (time to 90% PCE retention) increases from ~ 750 h for the pristine device to ~ 1800 h for the BPT device, consistent with experimental reports of >1000 h stability.

Comparative screening of passivators

To demonstrate predictive capability, we screened several sulfur-containing passivators (Table 6). Molecules with stronger Pb–S interactions and additional steric/hydrogen-bonding features exhibit larger migration barrier increases. BPT shows the highest ΔE_a (0.17 eV), diffusivity reduction (718-fold), predicted PCE (22.6%), and T_{90} (1800 h).

Table 6

Comparative screening of sulfur-containing passivators

Additive	MW, g/mol	ΔE_a (Γ), eV	D Reduction	Predicted PCE, %	T_{90} , h
Thiourea	76.1	0.11	68	22.8	780
Thioacetamide	90.1	0.13	95	23.1	920
Phenylthiourea	152.2	0.15	180	23.3	1150
BPT	318.4	0.17	718	22.6	1800
N-(o-Methoxyphenyl)thiourea	288.3	0.16	245	23.4	1380

The reported diffusivity reductions in Table 6 are relative estimates obtained under the assumption $D_0\approx\text{const}$ and reflect the contribution of ΔE_a to the suppression of ionic mobility.

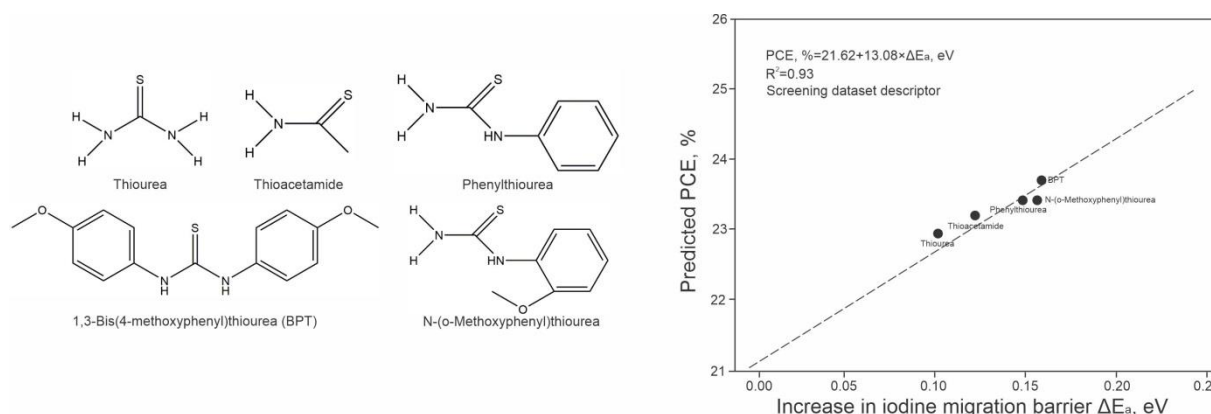


Figure 3. a) Molecular structures of the studied sulfur-containing passivators: thiourea, thioacetamide, phenylthiourea, N-(o-methoxyphenyl)thiourea, and 1,3-bis(4-methoxyphenyl)thiourea (BPT). b) Relationship between the increase in the iodide migration barrier (ΔE_a) serves as a descriptor for this screening data set and should not be interpreted as a universal quantitative relationship.

To demonstrate the predictive power of the developed multiscale approach, a comparative screening of a series of sulfur-containing molecules capable of coordinating with uncoordinated Pb^{2+} sites on the perovskite surface was conducted. Figure 3, a shows the molecular structures of the studied passivators, including thiourea, thioacetamide, phenylthiourea, N-(o-methoxyphenyl)thiourea, and BPT. A key structural feature of all selected molecules is the presence of a thiocarbonyl group ($\text{C}=\text{S}$), which acts as an electron density donor when interacting with defects in the perovskite lattice.

The calculation results presented in Figure 3, b) reveal a clear positive correlation between the increase in the iodide vacancy migration barrier (ΔE_a) and the predicted power conversion efficiency (PCE) of solar cells. The linear fit of the data is described by the equation $\text{PCE}(\%) = 21.62 + 13.08 \times \Delta E_a, \text{ eV}$ with a high coefficient of determination of $R^2 = 0.93$. This indicates that, within this data set, an increase in the energy barrier to ion migration is a reliable descriptor predicting improved photovoltaic performance of the device.

Among the molecules studied, BPT exhibits the largest increase in migration barrier ($\Delta E_a = 0.16\text{--}0.17$ eV) and the highest predicted PCE (22.6%). BPT's superiority over simpler analogs, such as thiourea ($\Delta E_a = 0.11$ eV, $\text{PCE} \approx 22.8\%$) and phenylthiourea, is explained by a synergistic effect. The presence of two bulky methoxyphenyl substituents in the BPT molecule not only creates additional steric hindrance to ion migration but also contributes to improved film morphology and grain boundary passivation due to enhanced van der Waals interactions. Thus, the combination of strong Pb-S electron interactions with optimal steric properties makes BPT the most effective passivator in the series under consideration, which is fully consistent with experimental data reported in the literature [22–26].

Conclusion

A multiscale DFT–COMSOL framework was developed to investigate BPT passivation in mixed-cation perovskite solar cells. DFT shows BPT interacts strongly with undercoordinated Pb sites, increasing migration barriers by up to 0.17 eV and suppressing defect-related electronic states. At the device scale, this translates to a PCE increase to 20.9% to 22.6%, a 35.1% reduction in temperature rise, and a 21.2% reduction in von Mises stress. The predicted T_{90} of 1800 h aligns with experimental stability. Comparative screening confirms that the combination of electronic, hydrogen-bonding, and steric characteristics in BPT makes it a highly effective passivator. Overall, this methodology provides a robust framework for the rational design of stable, efficient perovskite solar cells.

Acknowledgments

This research was supported by the Basic Fundamental Program of the Academy of Sciences of the Republic of Uzbekistan, the Uzbekistan–Turkey joint project funded by the Ministry of

Higher Education, Science and Innovation of the Republic of Uzbekistan (Grant No. AL-9825036056 “Developing efficient monolithic tandem silicon/perovskite cells”).

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