

RESEARCH ARTICLE OPEN ACCESS

Bright and Durable Copper-Iodide-Based Nanowire Scintillators

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Received: 25 May 2026 | **Revised:** 14 July 2026 | **Accepted:** 21 July 2026

Keywords: copper(I)-iodide | detection limit | light yield | nanowire | scintillator

ABSTRACT

The increasing demand for high-speed X-ray imaging requires scintillators with high light yield, rapid decay, and structural stability. Metal halide nanowires (NWs) have emerged as promising candidates due to their distinctive optical properties, high surface-area-to-volume ratio, high light yield, and high spatial resolution. However, their practical application is hindered by complex synthesis routes and performance degradation during the liquid–solid phase transition. Here, using CsCu₂I₃ NWs as a model system, we develop a streamlined low-temperature crystallization synthesis method and further introduce a surface protective agent strategy that significantly enhances scintillation performance. Through the use of tailored protective agents, the photoluminescence quantum yield of NWs increases from 12.78% to 21.65%, while the X-ray light yield improves by approximately ninefold, reaching $\sim 77,500$ photons MeV^{−1}. The optimized scintillator achieves a low detection limit of 59.20 nGy_{air}·s^{−1}, which is approximately 93-fold lower than the typical dose rate of standard medical X-ray diagnostics. Identical SPA treatment delivers uniform luminescence improvement across zero- and one-dimensional copper halide systems, confirming the generalizable regulatory effect of the proposed ligand coordination framework. This efficient and scalable approach not only advances nanowire-based scintillators but also provides a generalizable pathway for stabilizing solution-processed nanomaterials and accelerating their commercial adoption.

1 | Introduction

Lead-free copper-iodide-based scintillators have emerged as promising alternatives to toxic lead-halide perovskites, which suffer from intrinsic environmental incompatibility, ambient structural instability, and severe self-absorption losses [1–3]. These copper-iodide compounds offer substantial atomic numbers, large Stokes-shifted emission, fast radiative decay, and

negligible persistent afterglow [4–7]. Nevertheless, their practical application is severely hindered by low light yields relative to benchmark scintillators, specifically thallium-doped cesium iodide (CsI:TI), the most commercially successful and widely deployed system, and bismuth germanate (BGO), a classical standard in high-energy physics [1–3, 5, 7]. Additional limitations include pronounced thermal quenching of self-trapped exciton (STE) emission and copper(I) ion (Cu⁺) oxidation coupled

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with iodine vacancy defects that create deep-level nonradiative recombination centers [8, 9]. Among copper-iodide polymorphs, CsCu_2I_3 and $\text{Cs}_3\text{Cu}_2\text{I}_5$ are the two most extensively investigated scintillator candidates, yet they differ on the metrics that ultimately matter for commercial deployment [6, 10]. The yellow STE emission of CsCu_2I_3 is near-optimally matched to the peak response of mainstream Si CMOS and a-Si TFT photodetectors used in flat-panel X-ray imagers, whereas the blue emission of $\text{Cs}_3\text{Cu}_2\text{I}_5$ requires either blue-sensitive photodetectors or wavelength-conversion layers that add system complexity. The one-dimensional (1D) covalent $[\text{Cu}_2\text{I}_3]^-$ chain framework of CsCu_2I_3 also delivers stronger ambient and humidity tolerance than the electrostatically packed zero-dimensional (0D) clusters of $\text{Cs}_3\text{Cu}_2\text{I}_5$, reducing encapsulation requirements during device integration. Notably, dimensional engineering of CsCu_2I_3 into single-crystalline nanowires (NWs) further leverages this intrinsic structural anisotropy to enable directional carrier transport, reduces grain-boundary scattering and surface defect densities through improved crystallinity, enhances carriers collection and light extraction efficiency via waveguiding effects, and enable polarization-sensitive detection together with flexible device integration, attributes unattainable in 0D nanocrystal counterparts [11]. However, critical challenges persist for CsCu_2I_3 NWs, including insufficient light yield for high-energy-resolution applications, difficulties in scalable growth of large-area high-quality crystals while suppressing Cu^+ oxidation, persistent thermal quenching of STE emission, and suboptimal energy resolution relative to established industrial-grade standards stemming from intrinsic bandwidth broadening and defect-mediated nonradiative pathways.

Although currently lagging in light yield and energy resolution relative to benchmark standards, rapid advances in heterovalent doping and nanostructure engineering are narrowing this performance gap, positioning CsCu_2I_3 as a preferred candidate for next-generation lead-free scintillation applications. These limitations are being addressed through monovalent cation doping (e.g., sodium ion enhancement of photoluminescence, photoluminescence Quantum Yield, PLQY, to 19.60%), surface passivation via nanocrystal modification to tune decay kinetics, and nanowire microstructure optimization to improve carrier transport and light extraction [12, 13]. Notably, single-crystal CsCu_2I_3 has achieved PLQY exceeding 15.70%, substantially surpassing the ~5% typically reported for nanowire systems [10]. However, enhanced nanowire luminescence does not render CsCu_2I_3 suitable for direct-conversion X-ray detectors, as its appreciable ionic conductivity, modest carrier mobility-lifetime ($\mu\tau$) product, and exciton-dominated recombination fundamentally favor indirect scintillation over direct charge-collection modes; the latter requires semiconductor-grade $\mu\tau$ products exceeding $10^{-4} \text{ cm}^2 \text{ V}^{-1}$ and efficient electron-hole pair separation under electric bias [14]. Yet practical deployment of 1D CsCu_2I_3 NW architectures remains severely constrained by defect-mediated nonradiative recombination, Cu^+ oxidation-induced lattice destabilization, and solvent volatility-driven morphological instability during the liquid-solid transition, challenges that conventional solvent optimization and post-synthetic purification strategies fail to adequately mitigate. This transient interval dismantles the stabilized surface microenvironment through three coupled failure modes: structural roughening, redox instability, and interfacial coordination collapse, mechanisms that prove particularly devastating for

ultrathin nanostructures with elevated surface-to-volume ratios. Consequently, developing robust surface protective-agent (SPA) coordination strategies that simultaneously enhance PLQY, operational stability, and X-ray scintillation performance has emerged as an urgent priority for bridging the gap from “synthesizable” to “deployable” materials and enabling scalable integration of high-quality copper-iodide-based nanowire scintillators.

Herein, we report a streamlined, SPA-mediated low-temperature crystallization (LTC) strategy for synthesizing high-quality CsCu_2I_3 NWs at 273 K and atmospheric pressure. By treating the liquid-solid transition as an active kinetic regime rather than a passive endpoint, we elucidate the underlying crystallization kinetics and coordination mechanisms through electronic structure simulations and controlled comparative experiments. Among ethanol, acetonitrile, methanol, and acetone evaluated as SPAs, ethanol was ultimately identified as the optimal SPA. This SPA establishes a comprehensive stabilization framework that concurrently addresses three aforementioned failure modes: (i) a structural stabilization layer that arrests dissolution-redeposition-driven shrinkage to preserve 1D morphological integrity; (ii) a redox stabilization layer that maintains locally reducing microenvironments to suppress $\text{Cu}^+ \rightarrow \text{Cu}^{2+}$ oxidation during solvent removal; and (iii) an interfacial coordination stabilization layer in which hydroxyl groups of ethanol molecules form weak coordination bonds with low-coordination Cu^+ surface sites, thereby reconstructing and passivating under-coordinated sites within a weakly acidic microenvironment. This universal, low-cost SPA-ethanol-mediated approach extends the liquid-solid transition window and yields mutually reinforcing performance gains. The photoluminescence quantum yield increases from 12.78% to 21.65%, roughly twofold above reported solution-processed benchmarks, while the X-ray scintillation light yield reaches approximately 77,500 photons MeV^{-1} , surpassing that of pristine CsCu_2I_3 dendritic single crystals (DCs) by nearly ninefold and achieving a detection limit of $59.20 \text{ nGy}_{\text{air}} \cdot \text{s}^{-1}$ (~93-fold below conventional medical diagnostic requirements). Although demonstrated for CsCu_2I_3 , this conceptual architecture, which engineers protective microenvironments to resolve structural, redox, and coordination instabilities in parallel, offers a transferable pathway for stabilizing diverse solution-grown nanomaterials with applications in electroluminescent devices, light-emitting diode or laser phosphors, X-ray imaging, real-time radiation detection, and beyond.

2 | Results and Discussion

2.1 | Theoretical Simulations and Experimental Investigation of Luminescence Enhancement Feature

The fundamental and systematic investigation of surface microenvironments governing the liquid-solid transition in nanomaterials (e.g., quantum dots, nanocrystals, NWs) remains critically important [15]. Here, we employ CsCu_2I_3 as a model system, given its substantial specific surface area and significant potential for developing low-toxicity, high-performance scintillators. Based on a comparative analysis of two distinct CsCu_2I_3 NW architectures, we reveal that rapid

solvent removal (*N,N*-dimethylformamide [DMF] and toluene) and compositional drift during the liquid–solid transition cause the collapse of the buffered interfacial microenvironment. This collapse exposes the nanomaterial surface to coupled structural, redox, and coordination instabilities, manifesting as compromised growth quality, reduced structural stability, and abundant surface defects [16, 17]. To suppress these coupled failure modes, an SPA-mediated strategy is employed to enhance the growth quality and structural stability while considerably reducing surface defects (Figure 1a).

Before performing specific synthesis, density functional theory (DFT) calculations were conducted to gain deeper insight into the effects of different SPAs interacting with CsCu₂I₃ NWs surface. The total density of states (DOS) and partial DOS of the (010) plane in CsCu₂I₃ single crystals, both with and without a vacancy defect (*V*_I), as well as with various SPAs, are illustrated in Figure 1b and Figure S1. The crystal structure of CsCu₂I₃ comprises [Cu₂I₃][−] anionic chains that are spatially surrounded and isolated by rows of Cs⁺ cations. The [CuI₄]^{3−} tetrahedra are edge-shared, forming a 1D [Cu₂I₃][−] double-chain structure [18]. To simulate the effects of halide vacancies and SPAs on the NWs, a 9-layer slab structure was constructed on the (010) plane of CsCu₂I₃ and verified to achieve good convergence. A *V*_I defect was deliberately introduced, exposing the Cu atom on the outermost layer. Four distinct SPAs were designed to adsorb onto the slab surfaces. The adsorption stability was evaluated using the following binding energy formula:

$$E_{\text{binding}} = E_{\text{total}} - E_{\text{layer}} - E_{\text{SPA}} \quad (1)$$

where E_{total} , E_{layer} , and E_{SPA} represent the total energy of CsCu₂I₃, the energy of the layer, and the energy of the isolated SPA in the calculation, respectively. Introduction of the SPAs effectively repairs this defect-induced electronic disturbance. The negative binding energies listed in Table S1 indicate that adsorption of all four SPAs on the *V*_I-defective CsCu₂I₃ (010) surface is thermodynamically favorable, with ethanol (−0.40 eV) and methanol (−0.50 eV) exhibiting the strongest interactions among the molecules examined. Crucially, these binding energies lie within the characteristic range of coordinative bonding (−0.8 to −0.1 eV) and are markedly more negative than typical physisorption energies (>−0.1 eV). Combined with the emergence hybridized states near the Fermi level in the DOS spectra, DFT calculations confirm that ethanol forms a coordinative surface interaction via Lewis acid–base coordination, in which lone-pair donation from the oxygen atom of ethanol to under-coordinated surface Cu⁺ sites passivates the vacancy-derived electronic disturbance. Electronic structure analysis further reveals that ethanol adsorption shifts defect-related states away from the Fermi level, restores the bandgap, and suppresses trap-assisted nonradiative recombination (Figure S1f). Moreover, the spin-polarized DOS shows that the vacancy-induced spin asymmetry is nearly eliminated after ethanol adsorption, in line with near-complete quenching of the 1 μ_B magnetic moment associated with the *V*_I defect. These results suggest that the passivation of spin-polarized defect states by SPA coordination is responsible for the experimentally observed suppression of surface-defect-mediated non-radiative recombination.

In CsCu₂I₃ crystal, charge delocalization of bands around the Fermi level predominantly occurs on the iodine (I) and copper (Cu) atoms. The valence band maximum (VBM) consists mainly I-5*p* orbitals, whereas the conduction band minimum (CBM) comprises a hybrid of Cs-6*s*, Cu-4*s* and I-5*p* orbitals. The bulk CsCu₂I₃ structure exhibits a bandgap consistent with experimental observations; however, the slab model presents a slightly larger bandgap of approximately 3.48 eV. Introducing *V*_I to the CsCu₂I₃ slab surface not only shifts existing surface states energies but also generates new surface states, indicating that *V*_I induces charge localization near the vacancy site. Consequently, the slab model bandgap decreases to 2.98 eV, and the spin-polarized calculations reveal a localized magnetic moment of 1 μ_B per *V*_I arising from the unpaired electron density at the defect (Figure S1e,h).

Comparison among the four SPAs reveals a clear structure–effect correlation. When ethanol is incorporated into CsCu₂I₃ (SPA-ET), it effectively neutralizes the 1 μ_B magnetic moment originating from *V*_I, as illustrated in Figures S1 and S2. The defect level positions lie significantly distant from the CBM. Moreover, ethanol addition as an SPA further enhances charge localization around the I vacancy, yielding a more pronounced charge distribution, compared to the absence of the SPA. Consequently, radiative transition of the STE effect exerts substantial influence on luminescence intensity [6, 9]. The effect of acetonitrile as an SPA parallels that of ethanol in eliminating the system magnetic moment; however, the acetonitrile enhancement effect is slightly less pronounced than that of ethanol. This can be attributed to defect levels at 1.34 and 1.53 eV above the Fermi level being farther from the CBM. The STE effect exhibits greater sensitivity to trap states located closer to the CBM, as these states compete more effectively with the radiative recombination process, leading to nonradiative decay of the excited state. In contrast to ethanol, methanol and acetone fail to fully eradicate vacancy-induced spin asymmetry. DFT calculations reveal persistent spin-up trap carriers near the Fermi edge in methanol-treated models, leaving the 1 μ_B magnetic moment only partially neutralized. These residual spin traps compete with STE radiative transitions, inherently limiting the theoretical luminescence efficiency of methanol-modified samples to approximately half that of their ethanol-treated samples. Specifically, SPA introduction selectively removes surface organic residues from CsCu₂I₃. Meanwhile, SPAs can form moderate coordination bonds with iodine vacancies. This synergy can appreciably passivate deep-level defects while reducing or eliminating the associated magnetic moment, thereby substantially inhibiting nonradiative recombination. Furthermore, magnetic moment elimination induces band structure reorganization, facilitating radiative recombination pathways. This interaction markedly improves crystals optical performance and stability.

The comprehensive growth processes of two quintessential CsCu₂I₃ perovskites microstructure, NWs and dendritic aggregates, were investigated using an innovative LTC method. Based on time-resolved morphological evolution, together with surface composition and crystalline structure analysis, the formation of CsCu₂I₃ without SPA (W/O-mediated CsCu₂I₃) proceeded through four sequential stages: seed crystal growth, initial nanowire epitaxial growth, nanowire shrinkage, and self-assembled epitaxial regrowth into DCs. During the shrinkage stage, the initially grown CsCu₂I₃ NWs became unstable owing

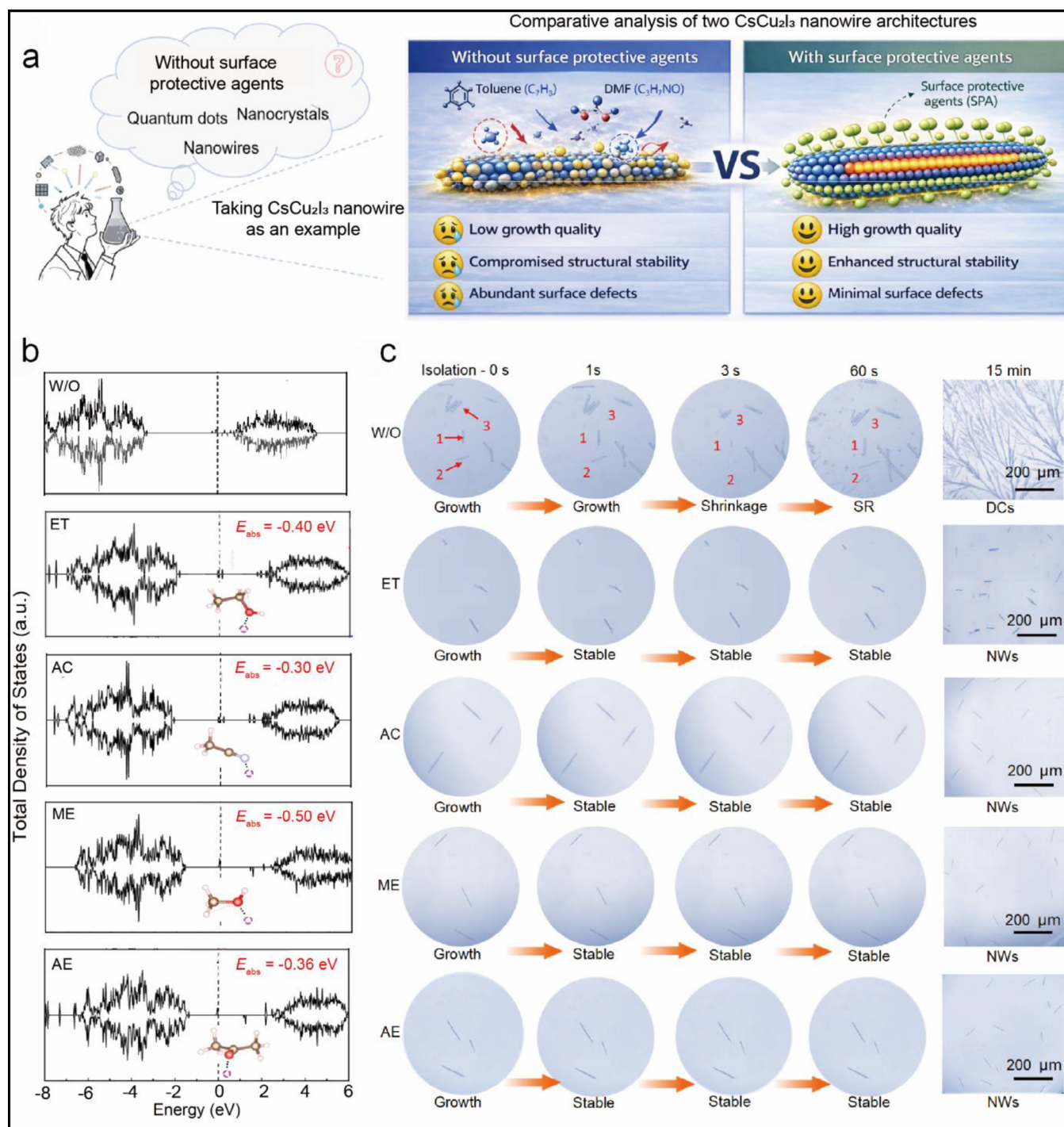


FIGURE 1 | Detailed schematics and dynamic images illustrating the formation procedures of CsCu_2I_3 DCs and NWs. (a) Schematic illustration of SPA-mediated strategy. (b) Calculated total density of states and partial charge densities for the slab model of CsCu_2I_3 crystal (the (010) plane) with one V_{I} defect and with ethanol, acetonitrile, methanol, and acetone as SPAs (ET: ethanol; AC: acetonitrile; ME: methanol; AE: acetone), respectively. All calculations were performed using the HSE functional. (c) Real-time growth processes of W/O-mediated CsCu_2I_3 DCs (Specimens 1–3) and SPA-mediated CsCu_2I_3 NWs, captured using an optical microscope. Specific growth stages of each specimen were recorded at intervals of 1 s, 3 s, 60 s, and 15 min.

to decomposition induced by excessive DMF and toluene on the nanowire surface, resulting in unstable nucleation and distinctive self-assembly behavior. The driving force for nanowire shrinkage stemmed from differential volatilization kinetics between DMF and toluene, as confirmed by time-resolved solvent evaporation measurements (Figure S3). Locally concentrated residual DMF

hinders directional nanowire growth and accelerates the dissolution of as-synthesized CsCu_2I_3 NWs. The SPA solvents (ET and ME) carry substantially higher pKa values (15.90 ± 0.40) than the control (DMF, -0.30 ± 0.40), endowing them with an intrinsic acid-buffering capacity that persists across all three crystallization stages (Figure S4). Tracking pH from neat solvent

through precursor dissolution to the toluene-added nanowire growth environment reveals that SPA systematically acidifies and stabilizes the local microenvironment (precursor pH 4–5.5 vs. 5.5–6 for neat DMF), remaining active at the crystal–solution interface rather than being expelled upon solvent addition (Figure S5). Benefiting from such interfacial acid–base regulation, SPA reconstructs the crystallization microenvironment via modulating solvent polarity and buffering interfacial acid–base equilibrium, which extends the nucleation induction period and decelerates crystallization kinetics. The consequence is visually unambiguous: under UV illumination, all SPA-mediated CsCu_2I_3 NWs emit markedly brighter and more uniform yellow light than the W/O control, whose faint luminescence reflects the unpassivated defects of an unmanaged liquid–solid transition (Figure S6) [19, 20]. To verify this growth procedure, precursor specimens were collected at appropriate intervals following toluene addition and monitored via real-time optical microscopy. The accelerated shrinkage stage was clearly captured in Figure 1c (Specimens 1–3), confirming the detailed real-time evolution of individual W/O-mediated CsCu_2I_3 NWs. The W/O-mediated CsCu_2I_3 NWs exhibited rapid shrinkage and even transient disappearance. Subsequently, with progressive DMF volatilization, the NWs gradually underwent secondary reconstruction (SR). Eventually, distinctive and abundant self-assembled dendritic CsCu_2I_3 single crystals with multiple branches, comprising numerous NWs arranged in a spoke-like configuration, were formed.

2.2 | Multifaceted Experimental Characterization of SPA-Mediated Stabilization Mechanisms

By precisely modulating the nanowire surface microenvironment, the reaction kinetics and thermodynamics are optimized, thereby enhancing both growth quality and structural stability. As shown in Figure 2a, SPAs are employed to effectively remove DMF and toluene residues from the surfaces of CsCu_2I_3 NWs. This step prevents the adsorption and coverage of precursors and reactants, which would otherwise alter the electronic structure of the nanowire surface, induce incomplete reactions, and potentially lead to oxidation. X-ray photoelectron spectroscopy (XPS) measurements were performed to analyze the surface chemical composition and valence states of CsCu_2I_3 . Figures S7–S9 and Figure 2b display the individual high-resolution energy spectra of CsCu_2I_3 , Cs 3d, I 3d, and Cu 2p species. The asymmetric peak of W/O-mediated CsCu_2I_3 DCs is deconvoluted into three peaks at approximately 930, 932.43, and 934.78 eV, attributed to $\text{I } 3p_{1/2}$, $\text{Cu}^+ 2p_{3/2}$, and $\text{Cu}^{2+} 2p_{3/2}$, respectively. The $\text{I } 3p_{1/2}$ core level overlaps with Cs^+ MNN Auger lines. Another peak is deconvoluted into two main peaks with binding energies at 952.13 and 953.80 eV, corresponding to $\text{Cu}^+ 2p_{1/2}$ and $\text{Cu}^{2+} 2p_{1/2}$, respectively [18, 21, 22]. The Cu^{2+} signal centered at 934.78 eV accounts for 14.59% of the total Cu spectral intensity, accompanied by distinct satellite peaks characteristic of Cu^{2+} species. This result confirms that a substantial portion of Cu^+ cations at the pristine surface has been oxidized to Cu^{2+} owing to the under-coordinated Cu centers adjacent to V_1 defects [23]. Following SPA addition to the precursor, the binding energies associated with $\text{Cu}^+ 2p_{1/2}$ and $\text{Cu}^+ 2p_{3/2}$ in the SPA-mediated CsCu_2I_3 NWs closely match those of the sample without SPAs. Moreover, Cu^{2+} signals are suppressed below the instrument's reliable detection limit; only

Cu^+ -dominated peaks at ~ 932.3 – 932.6 eV are observed, and no resolvable Cu^{2+} satellite features are detected. These XPS results verify that the intrinsic reducing microenvironment introduced by SPA additives fully inhibits oxidation of Cu(I) throughout the crystallization process.

Additionally, peaks centered at ~ 532 and 286.18 eV are attributed to C=O and C–O–C, respectively (Figure 2c and Figure S9). Notably, the O 1s signals of adsorbed molecules appear at 531.37–531.70 eV, which are substantially lower than the O 1s position of free ethanol (~ 533.5 eV). This negative binding energy shift originates from the donation of oxygen lone-pair electrons to under-coordinated surface Cu^+ sites, consistent with the DFT density-of-states calculations. Compared with the pristine sample bearing CuO_x -derived O 1s and Cu^{2+} satellite peaks, all solvent-treated specimens only exhibit organic oxygen features without spectral fingerprints of free ethanol. Meanwhile, the complete disappearance of Cu^{2+} signals in Cu 2p spectra further excludes surface oxidation and verifies strong interfacial interactions between solvent molecules and the substrate. Collectively, these XPS characterizations prove that solvent molecules are chemically immobilized on the CsCu_2I_3 surface through Cu–O coordinative bonding rather than weak physisorption. In conclusion, the disappearance of Cu^{2+} features, the reduction of under-coordinated I^- sites, and the emergence of Cu–O coordination signatures constitute three converging experimental lines of evidence for the coordination-based passivation of V_1 defects at the CsCu_2I_3 surface.

These observations demonstrate that SPAs effectively prevent Cu^+ oxidation and ensure uniform crystal growth throughout. Figure 2d summarizes the overall elemental content analysis by XPS. Treatment with the four solvent molecules selectively lowers the total surface organic content (C+O+N), with the ethanol-treated sample delivering the most significant reduction of 62.0% among all tested systems. Specifically, carbon content exhibits the sharpest relative decline (–74.3%), indicative of thorough stripping of carbon-laden DMF and toluene residual impurities. Nitrogen concentration decreases moderately (–42.6%), a trend consistent with the selective displacement of DMF molecules bearing N-CHO functional groups. In stark contrast, oxygen atomic proportion only undergoes a mild relative drop (–37.8%). This modest oxygen loss stems from two competing interfacial effects: the elimination of surface CuO_x oxide species, alongside partial retention of ethanol oxygen anchored via Cu^+ -O coordinative interactions, fully consistent with the interfacial bonding mechanism supported by prior XPS and DFT analyses.

However, XPS is a surface-sensitive technique probing primarily the outermost few nanometers of both W/O- and SPA-mediated CsCu_2I_3 . In contrast, solid-state nuclear magnetic resonance (SSNMR) serves as a powerful complementary method for bulk compositional analysis, offering valuable insights into the local nuclear environment within the structure, particularly for quantifying residual solvent content. Consequently, ^1H SSNMR measurements were conducted on W/O- and SPA-mediated CsCu_2I_3 (Figure S10). The pristine W/O sample exhibits characteristic ^1H signals of residual DMF and toluene trapped within the as-grown CsCu_2I_3 , whereas these residual-solvent signals are markedly suppressed in the SPA-treated samples, indicating that

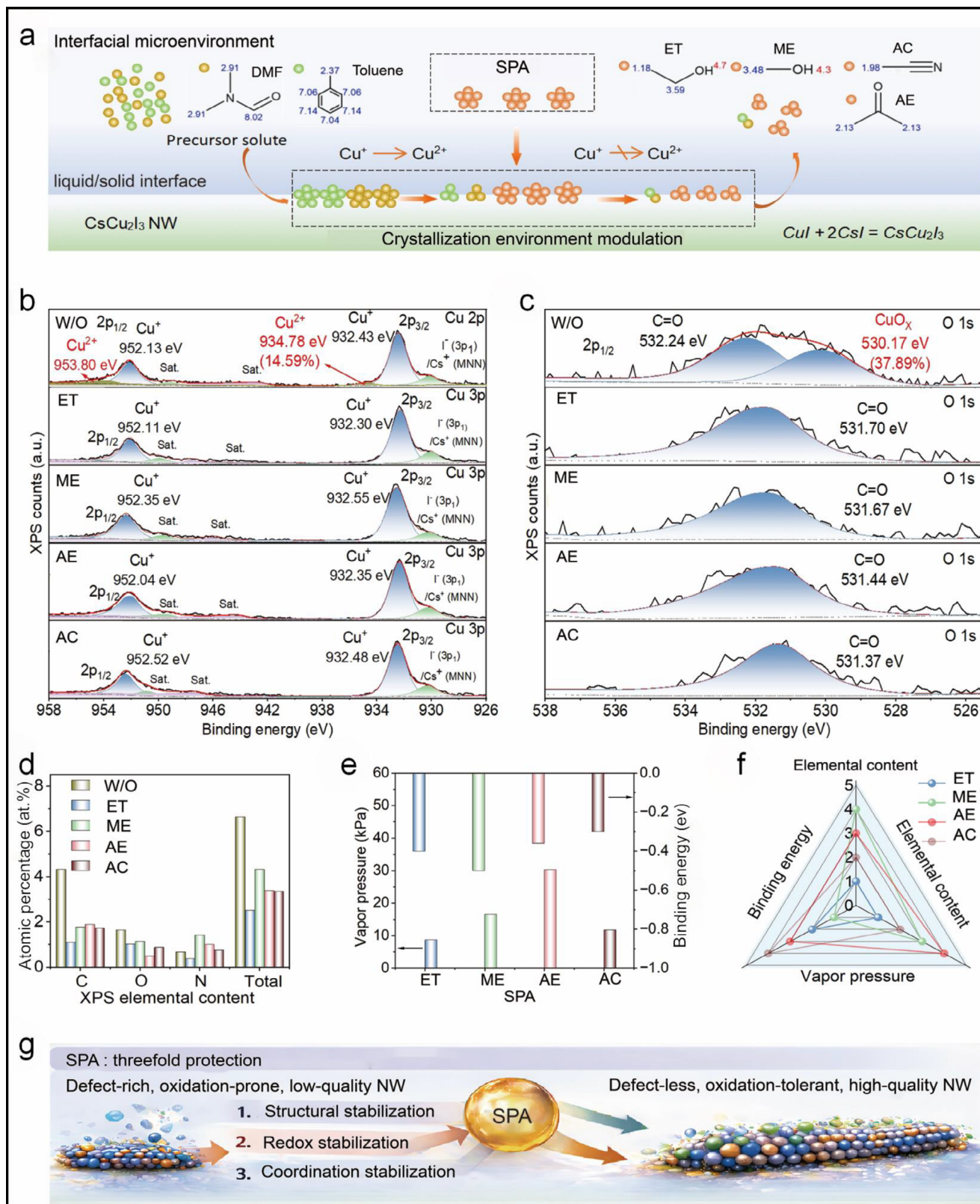


FIGURE 2 | Comprehensive multifaceted experimental characterization of SPA-mediated surface microenvironment optimization. (a) Schematic illustration of interfacial microenvironments and proposed reaction processes. High-resolution XPS energy spectra of (b) Cu 2p and (c) O 1s for CsCu₂I₃ NWs. (d) Comprehensive elemental analysis of CsCu₂I₃ by XPS. (e) Vapor pressure of solvents used in this study at 25°C (top panel) and binding energies between CsCu₂I₃ (010) surface with one V₁ and various SPAs, including ET, AC, ME, and AE. (f) Radar chart evaluating performance across three metrics: XPS elemental content, saturated vapor pressure, and calculated binding energy. (g) Schematic illustrating three concurrent protective functions by SPA.

the SPAs selectively remove the DMF and toluene impurities during nanowire growth. Moreover, the SPA-treated samples display new resonances at chemical shifts characteristic of the corresponding SPA molecules, accompanied by pronounced peak broadening relative to their free-molecule counterparts. The peak broadening reflects a distribution of local chemical environments experienced by the SPA molecules upon anchoring at the nanowire surface, consistent with a chemisorptive Cu-O coordination rather than a free physisorbed state. These SSNMR observations support a model in which SPA molecules remain chemically anchored at the CsCu_2I_3 surface, providing bulk-sensitive evidence that complements the surface-sensitive XPS analyses and independently corroborates the coordinative binding mechanism. Figure 2e, Figure S11, and Table S2 summarize the vapor pressure of the solvents that were used in this study at 25°C. Vapor pressures were calculated using the Antoine equation: $\log P = A - (B/(T + C))$, where P is the vapor pressure (atm) at temperature T (K); the values were then converted to kPa by multiplying by 1.33×10^{-1} . Constants were obtained from *Yaws' handbook of Thermodynamic and Physical properties of Chemical Compounds* [24]. Among the four candidate SPAs investigated, ethanol exhibits the lowest saturated vapor pressure (8.72 kPa). Critically, this slow evaporation rate not only prolongs the solvent-surface interaction but also facilitates the controlled removal of surface impurities (e.g., DMF and toluene), preventing them from being encapsulated within the crystal lattice. Complementing electronic effects, solvent volatility governs interfacial dynamics. Methanol exhibits a saturated vapor pressure nearly twice that of ethanol at 25°C. Its rapid volatilization drastically curtails surface residence time, precluding the formation of a persistent, homogeneous coordination layer. In contrast, ethanol combines sufficient chemisorption strength to fully neutralize spin and electronic defects with lower volatility, maintaining stable interfacial ligand coverage throughout the whole crystallization process.

Overall, through comprehensive analysis of individual elemental content, saturated vapor pressure, and computational binding energy, we established an effective radar chart to visualize the CsCu_2I_3 surface microenvironment. As shown in Figure 2f, CsCu_2I_3 NWs modified by these SPAs exhibit more pronounced synergistic effects among these three parameters, which significantly influence the surface microenvironment. Stronger interactions between SPAs and the CsCu_2I_3 NWs surface alter the physical state of adsorbed species, electronic structure, and surface chemical properties. These modifications positively affect nanowire crystal quality and luminescence efficiency and are quantitatively supported by the convergence of the DFT-calculated binding energies and the XPS observations of Cu^{2+} elimination and reduced under-coordinated I sites, which establish a coherent picture in which SPA coordination passivates the V_I defects at the nanowire surface. This finding provides valuable insights into the mechanism by which SPAs influence NWs, establishing three concurrent protective actions: structural stabilization, redox stabilization, and coordination stabilization, thereby maximizing performance of nanowire-based materials and devices (Figure 2g and Figure S12). This approach also offers a promising platform for designing and controlling nanowire surface microenvironments to achieve enhanced functionality.

2.3 | Tailored Nanostructure Evolution and Microstructural Characterization

X-ray diffraction (XRD) analysis was performed on five CsCu_2I_3 single-crystal morphologies to investigate this peculiar phenomenon (Figure S13). Interestingly, coordination of the four SPAs did not induce any structural changes. The XRD patterns of W/O- and SPA-mediated CsCu_2I_3 NWs closely matched the orthorhombic structure of CsCu_2I_3 (Cmcm, JCPDS NO. 45-0076), consistent with previous reports [18, 21, 22]. Compared to W/O DCs, all SPA-treated NWs show narrower diffraction peak full-width at half-maximum (FWHM) and lower microstrain (ϵ), indicating the effective release of residual lattice strain and a concomitant enhancement in crystalline quality (Table S3). To investigate the morphological and crystallographic evolution induced by the ethanol treatment, comprehensive structural characterization of both W/O- and ethanol-mediated CsCu_2I_3 NWs was performed by transmission electron microscopy (TEM) equipped with an energy-dispersive X-ray (EDX) spectrometer. As shown in Figure 3a,b, both samples exhibit well-defined 1D nanowire morphology. Notably, surfaces of the interlaced NWs featured numerous sprouts and junctions, which facilitated the self-assembly growth of DCs. The average diameter of the ethanol-based NWs (~322.00 nm) is slightly reduced, compared to the W/O-based counterparts (~372.00 nm), suggesting that the ethanol-mediated process promotes moderate surface structural reorganization. Furthermore, high-resolution TEM images of CsCu_2I_3 NWs revealed clear lattice fringes with interplanar spacing of approximately 0.34 nm, consistent with the (221) plane of CsCu_2I_3 single crystals [11, 21, 22]. This observation aligns well with XRD results. Corresponding selected area electron diffraction (SAED) patterns display distinctive, sharp diffraction spots, further confirming the preferred single-crystalline nature. Meanwhile, elemental mapping (Figure 3c and Figure S14) confirms uniform distribution of Cs, Cu, and I throughout nanowire cores in both samples, whereas light elements C, O, and N are preferentially located at nanowire surfaces, consistent with adsorbed organic species. In contrast, Figure 3d reveals negligible contents of C and N. Additionally, EDS line-scan profiles (the insets of Figure 3c,d) further corroborate these findings: the I, Cs, and Cu signals are colocalized and confined within the nanowire cross-section, whereas C, N, and O signals exhibit peripheral enrichment. Notably, the ethanol-treated sample displays more uniform elemental distribution and reduced C, N, and O signal intensities at the surface, implying partial removal or passivation of surface oxide species.

To quantitatively probe the elemental homogeneity and Cu valence state distribution at the macroscopic scale, XPS 2D mapping was employed (Figure 3e,f and Figure S15). The Cs distribution remains relatively more spatially uniform in ET-mediated samples across the $100 \times 100 \mu\text{m}^2$ mapped area, confirming greater structural integrity. In contrast, the I distribution in the W/O-based sample displays pronounced spatial inhomogeneity, whereas the ET-based sample exhibits a markedly more homogeneous I signal, indicating that ET treatment appreciably improves halide ion uniformity and partially suppresses I-vacancy-related defects. Regarding Cu valence states, both Cu^+ and Cu^{2+} are present in the W/O-based sample with spatially inhomogeneous distribution and appreciable Cu^{2+} signal across the mapped

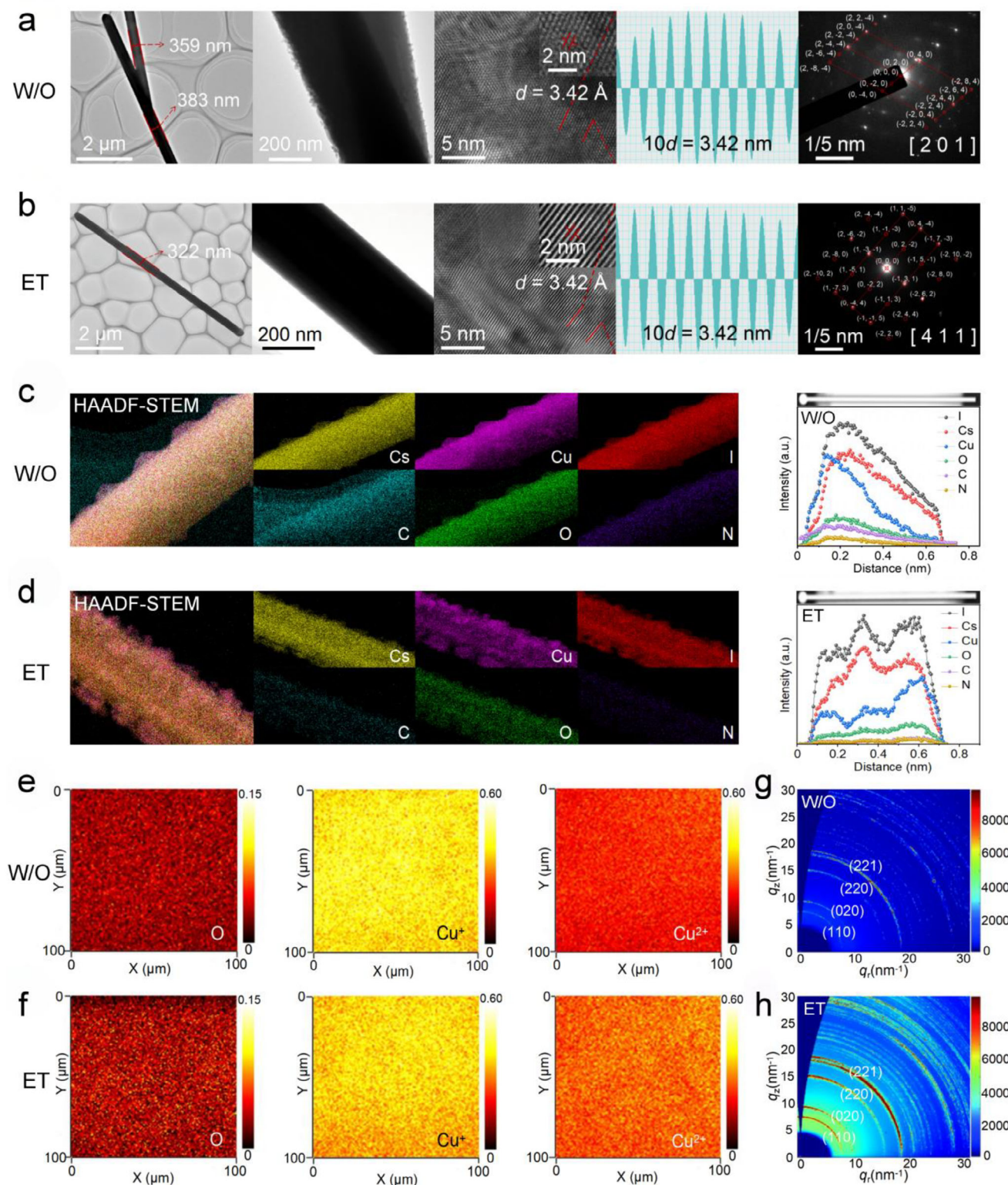


FIGURE 3 | Illustration of nanostructure evolution and verification of microstructural characteristics in CsCu_2I_3 DC and CsCu_2I_3 NWs. (a,b) TEM images, HRTEM images, and corresponding SAED patterns of the W/O- and SPA-mediated CsCu_2I_3 NW. Insets show magnified lattice regions. (c,d) The high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images of Cs, Cu, I, C, O and N for individual W/O- and SPA-mediated CsCu_2I_3 NW. Insets on the bottom right EDS line-scan profiles. (e,f) Spatial distribution maps and (g,h) 2D GIWAXS patterns of W/O-mediated CsCu_2I_3 DCs and SPA-mediated CsCu_2I_3 NWs with ethanol. Scattered rings at $q \approx 7, 10, 16, \text{ and } 19 \text{ nm}^{-1}$ corresponding to (110), (020), (220), and (221) diffractions planes of the CsCu_2I_3 crystal, respectively.

area. In contrast, the ET-based sample exhibits a markedly more homogeneous Cu^+ distribution alongside a pronounced reduction in Cu^{2+} content. Critically, this Cu^{2+} suppression persists through toluene washing and ambient drying, confirming that ethanol forms a quasi-stable coordinative interaction with surface Cu^+ sites rather than transient physisorption. This processing resilience highlights the robustness of the Cu^+ -O bond in suppressing surface oxidation. The O distribution maps mirror this trend, with the ET-based sample showing a lower and more uniform O signal, consistent with reduced surface oxidation. The crystallographic structures of CsCu_2I_3 single crystals were further investigated using Grazing Incidence Wide-Angle X-ray Scattering (GIWAXS) measurements. Figure 3g,h and Figure S16 compare the 2D GIWAXS patterns of W/O- and the four SPA-mediated CsCu_2I_3 NWs. The diffraction profiles were similar. Among these, the SPA-ET-mediated CsCu_2I_3 NWs exhibited the brightest and sharpest scattered rings, indicating enhanced crystallinity. This conclusion was corroborated by comparing the azimuthally integrated intensities of the scattered rings at $q \approx 7, 10, 16$, and 19 nm^{-1} , corresponding to the (110), (020), (220), and (221) diffraction planes, respectively (Figure S17). Here, q represents the scattering vector ($q = 4\pi\sin(\theta)/\lambda$), consistent with the XRD patterns. The ET-based sample displays significantly enhanced peak intensities, indicative of improved long-range crystalline order and reduced defect density, consistent with the effective passivation mechanism.

2.4 | Diverse Stability Variation Behaviors Under PL and Radioluminescence (RL) Irradiation

To elucidate the emission mechanism, the luminescence properties of a series of pristine CsCu_2I_3 DCs and SPA-mediated CsCu_2I_3 NWs were investigated under UV excitation and X-ray irradiation, respectively. RL is triggered by high-energy radiation (X-ray) with photon energies several orders of magnitude greater than those employed in PL. For reference, a commercially available BGO inorganic scintillator was selected. Figure 4a illustrates the presence of multiple electrons in the nucleus of CsCu_2I_3 perovskites. Incident X-ray photons are initially absorbed by the heavy atoms in CsCu_2I_3 perovskites, predominantly through the photoelectric effect and inelastic Compton scattering. This process ejects a large number of high-energy “hot” electrons and deep holes [7, 9, 25]. These electrons rapidly thermalize, generating numerous energetic secondary electrons that subsequently relax to the conduction band bottom. Eventually, they are captured to form STEs for recombination. STE luminescence is a distinctive fluorescence property of low-dimensional metal halide perovskites. Figure 4b,c and Figure S18 reveal that CsCu_2I_3 DCs exhibit a broad yellow RL emission with a peak wavelength at 574 nm, a broad photoluminescence excitation (PLE) spectrum peaking at $\sim 320 \text{ nm}$, and a broad yellow PL emission with a peak wavelength of 556 nm (FWHM of 106 nm). The large Stokes shift ($\sim 230 \text{ nm}$), attributed to STEs, results in negligible self-absorption, which is advantageous for scintillation light output [4–7, 26–28]. Figure S19 displays the excitation power-dependent RL spectra of CsCu_2I_3 , indicating that the emission intensity increases with increasing power under X-ray irradiation (excitation power: 0.5–12 W). Moreover, the spectral profiles of the emission peak under UV excitation are consistent with those

under X-ray irradiation, confirming that the final luminescence stage of X-ray luminescence originates from the same radiative recombination pathway under both X-ray irradiation and UV excitation; both emit light through STEs. Due to the soft crystal lattice nature of CsCu_2I_3 perovskites and strong electron–phonon coupling, free excitons are rapidly self-trapped to form STEs under UV excitation. This process originates from excited-state structural reorganization caused by Jahn–Teller distortion [21, 22, 29, 30]. Ultimately, the strongly Stokes-shifted broadband yellow emission results from a radiative transition from the STE state to the ground state.

Remarkably, the introduction of SPAs significantly enhances the emission intensities under both X-ray and UV excitation, while peak positions remain almost unchanged regardless of the specific SPA employed. Notably, the emission enhancement of ethanol-mediated CsCu_2I_3 NWs is nearly threefold higher than that of pristine CsCu_2I_3 DCs under X-ray excitation and almost nine-fold higher than that of the commercially available BGO inorganic scintillator. Under UV excitation, the emission intensity of CsCu_2I_3 NWs coordinated with either ethanol or acetonitrile is substantially greater (>20 -fold) than that of pristine CsCu_2I_3 DCs. Specifically, Figure S20 and Table S4 demonstrate a substantial improvement in PLQY from 12.78 % (CsCu_2I_3 DCs) to 21.65 % (ethanol-mediated CsCu_2I_3 NWs), surpassing previously reported values for CsCu_2I_3 . Thus, SPAs can effectively modulate the luminescence kinetics of STEs. Figure S21 shows the PL decay curves collected under 327 nm excitation, which are fitted with a biexponential function to calculate an average PL lifetime (τ_{ave}) 14.35 μs for ethanol-mediated CsCu_2I_3 NWs at room temperature, exceeding the τ_{ave} of 9.32 μs for CsCu_2I_3 DCs. These results confirm that SPAs reduce nonradiative recombination caused by surface defects, consistent with the significantly enhanced PLQYs. To further understand the origin of the enhanced PLQY, the radiative (k_r) and non-radiative (k_{nr}) recombination rate constants of the STE emission were calculated from the absolute PLQY and τ_{ave} using $k_r = \text{PLQY}/\tau_{\text{ave}}$ and $k_{\text{nr}} = (1 - \text{PLQY})/\tau_{\text{ave}}$, as summarized in Table S5. Compared with the pristine CsCu_2I_3 DCs, the ET NWs exhibit a modest increase in k_r by 10.2% and a pronounced decrease in k_{nr} by 41.7%. This indicates that SPA passivation contributes to the PLQY enhancement not only through a moderate acceleration of the radiative transition but, more importantly, through a substantial suppression of surface-defect-mediated non-radiative recombination, which is in good agreement with the theoretical analysis in Figure 1b. The pronounced k_{nr} suppression, together with the prolonged τ_{ave} and elevated PLQY, provides quantitative confirmation of the surface passivation mechanism proposed above. Strongly bound ethanol and acetonitrile chemically coordinate under-coordinated Cu atoms via Lewis acid-base interactions, near-completely compensating unpaired electrons, eliminating the vacancy-induced magnetic moment, and shifting defect trap states away from the CBM. This suppresses non-radiative decay and enables dominant STE emission, consistent with the experimentally observed PL peak position and elevated PLQY. In contrast, methanol and acetone only partially quench the spin moment, yielding comparatively weaker luminescence. Detailed adsorption geometries, charge transfer information, and iodine vacancy formation energies are provided in the Supporting Information (Figures S22–S24, Tables S6–S9).

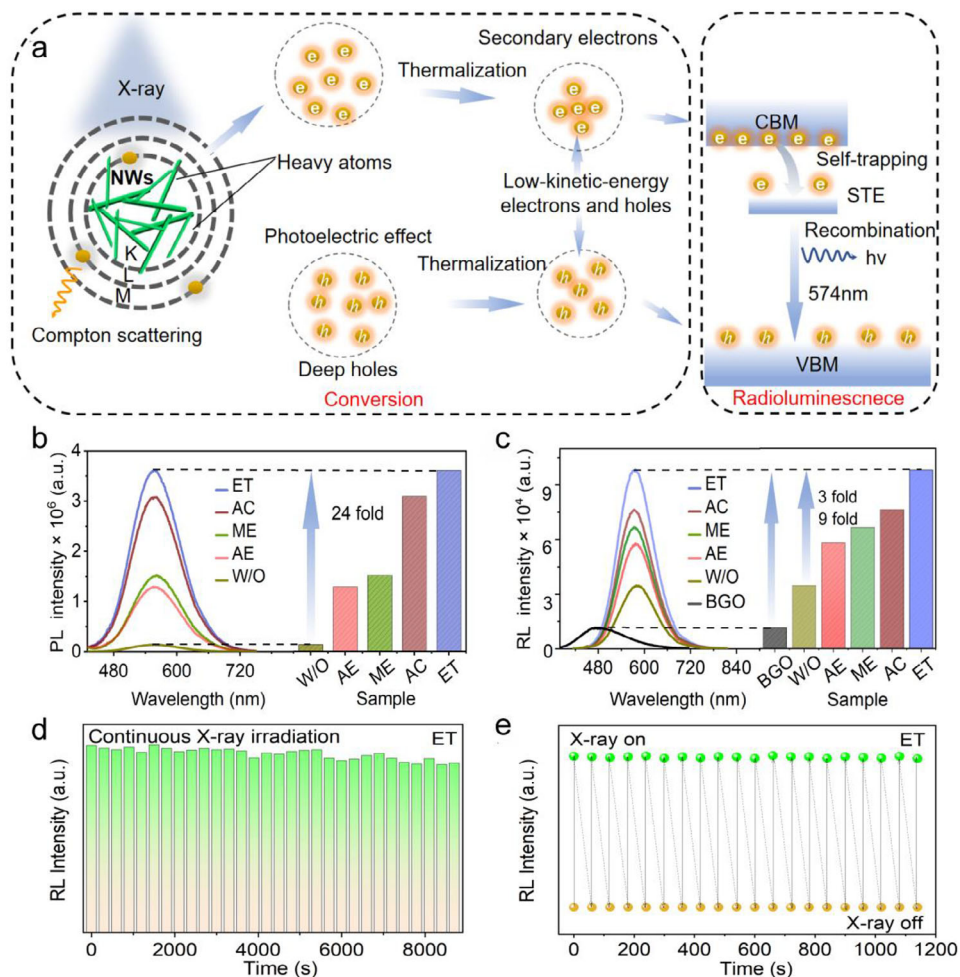


FIGURE 4 | Investigating the scintillation mechanism and diverse stability behaviors of CsCu₂I₃ NWs. (a) Schematic illustration of the scintillation process in CsCu₂I₃ scintillators. The CBM and VBM denote the conduction band minimum and valence band maximum, respectively. (b,c) Emission spectra of CsCu₂I₃ DCs and CsCu₂I₃ NWs treated with different SPAs (ethanol, acetonitrile, methanol, acetone) under the excitation of X-rays and UV light, respectively. BGO refers to the commercially available Bi₄Ge₃O₁₂ inorganic scintillator crystal. (d) Stability of RL intensity of CsCu₂I₃ NWs under continuous X-ray irradiation for 8700 s at a dose rate of 22.90 μGy_{air}·s⁻¹. (e) Radiation stability of CsCu₂I₃ NWs with repeated cycles of X-ray excitation, with a time interval of 60 s between cycles.

Given the similar properties of CsCu₂I₃ NWs treated with different SPAs, ethanol-mediated CsCu₂I₃ NWs were selected as the representative sample for subsequent analysis. The stability of a scintillator is a crucial parameter describing its radiation resistance. The stability against X-ray illumination was assessed by monitoring changes in RL intensity under continuous X-ray irradiation at a dose rate of 22.90 μGy_{air}·s⁻¹ for 8700 s. As shown in Figure 4d, only minor fluctuations in RL intensity were observed, indicating virtually no degradation under prolonged X-ray exposure. This clearly demonstrates the long-term stability of CsCu₂I₃ NWs for X-ray scintillation applications. Moreover, the CsCu₂I₃ NWs scintillator also exhibited excellent repeatability and photostability under repeated cycles of X-ray exposure (Figure 4e). To evaluate the effects of storage and UV light exposure on the structure and optical properties of CsCu₂I₃, its photostability, moisture resistance, and thermal stability were investigated. A pigeon pattern was drawn using a suspension of ethanol-mediated CsCu₂I₃ NWs precursor solution. After natural drying, the drawing disappeared under daylight but became visible as yellow fluorescence under 254 nm UV lamp irradiation

after storage for 10 months in ambient atmosphere (Figure S25). The optical properties exhibited remarkable long-term air stability, with no significant change in fluorescence brightness. Moisture and thermal stability tests were conducted by storing the CsCu₂I₃ NWs under 85% relative humidity (RH) and at a constant temperature of 85°C. Notably, the PL intensities of the CsCu₂I₃ NWs exhibited negligible change, indicating remarkable stability (Figures S26 and S27). This stability can be attributed to the robust Cu-I bonds within the unique 1D crystal structure [31].

The photostability of treated CsCu₂I₃ without any encapsulation or protection was further tested under continuous UV irradiation with 23 mW cm⁻² for 50 h (25°C, 40% RH). Remarkably, the ethanol-mediated CsCu₂I₃ NWs maintained a PLQY as high as 13% over 50 h, which was higher and more stable than previously reported values for CsCu₂I₃ (typically below ~10 %) [4, 31–33]. To more accurately assess thermal stability, the variation in PL emission intensity and Commission Internationale de L'Eclairage (CIE) chromaticity coordinates of the CsCu₂I₃ NWs was monitored during consecutive heating–cooling cycle

(303–373–303 K), as shown in Figures S28–S30. The CsCu_2I_3 NWs displayed reproducible PL behavior throughout these heating–cooling cycles. Concurrently, optical microscope images revealed that the original fluorescence brightness remained nearly uniform after four successive heating–cooling cycles. Therefore, the negligible decrease in emission intensity, color stability, and minimal change in CIE chromaticity coordinates at equivalent temperatures indicate high reversibility, excellent repeatability, and superior thermal stability and tolerance.

To gain deeper insights into the photophysical properties and electron–phonon interactions, temperature-dependent PL spectra were measured under xenon lamp excitation at 327 nm (Figure S30c). As the temperature increased, the integrated PL intensity gradually decreased while the FWHM simultaneously broadened. This behavior could be attributed to enhanced coupling between phonons and excitons at elevated temperatures, which activated nonradiative recombination processes [34]. The exciton binding energy (E_b) was determined from the Arrhenius plot of the corresponding integrated PL intensity for SPA-mediated CsCu_2I_3 NWs (Figure S30d). The calculated E_b value of STE was 430.60 ± 12.60 meV, significantly higher than that of conventional CsCu_2I_3 perovskites [35]. This high binding energy facilitates the transition of free excitons across the potential barrier to the STE state, thereby enhancing the STE emission and achieving higher PLQY. Furthermore, the Huang–Rhys factor (S) and phonon frequency $\hbar\omega_{\text{phonon}}$ were derived from the temperature-dependent FWHM. The S value was determined to be 39.29, substantially exceeding those of most traditional emission materials, such as ZnSe (0.31) [36], $\text{K}_2\text{NaScF}_6\text{:Cr}^{3+}$ (2.96) [37], ScF_3 (3.01) [38], and CsPbBr_3 (3.49) [39]. This remarkably high S indicates the soft crystal nature of SPA-mediated CsCu_2I_3 NWs and the facile formation of STEs within this material. As displayed in the time-dependent PL spectra of ethanol-treated NWs (Figure S31), negligible attenuation of PL intensity is observed over continuous aging durations ranging from 2 to 50 h, with nearly overlapping spectral profiles maintained across all time points. This result solidifies that the triple SPA protective framework sustains structural, redox and interfacial coordination stability over long service times.

2.5 | Comprehensive Applications of High-Resolution X-Ray Scintillation Imaging

The characterization results indicate that SPA-mediated CsCu_2I_3 NWs hold considerable promise as scintillators for X-ray phase-contrast imaging. Subsequently, the CsCu_2I_3 -based scintillators for X-ray imaging were evaluated using the prototype projection setup illustrated in Figure 5a. High-resolution X-ray images of a semiconductor chip (2×2 cm) and a small electronic component, acquired using the SPA-mediated CsCu_2I_3 NWs scintillation platform with a standard digital camera and a 50 keV X-ray source, are presented in Figure 5b,c. The internal configuration of the chip is not visible to the naked eye; however, owing to the substantial difference in X-ray attenuation between the conductive tracks and the silicone resin, the conductive tracks within the chip can be clearly discerned at an X-ray dose rate of $62.20 \mu\text{Gy}_{\text{air}}\cdot\text{s}^{-1}$. This exceptional X-ray imaging performance is attributed to the negligible self-absorption, high PLQY, and low detection limit of SPA-mediated CsCu_2I_3 NWs. Such high-contrast imaging

demonstrates the potential of SPA-mediated CsCu_2I_3 NWs as a promising candidate for X-ray radiography applications [40–42]. To evaluate the spatial resolution of the scintillation screen, a standard X-ray resolution test pattern was employed. The spatial frequency of the output, expressed in line pairs per millimeter ($\text{lp}\cdot\text{mm}^{-1}$), represents the modulation transfer capability of the input signal. Consequently, the image resolution achieved with the CsCu_2I_3 NWs scintillator reaches nearly $8 \text{ lp}\cdot\text{mm}^{-1}$ (right), surpassing that W/O-mediated CsCu_2I_3 DCs at approximately $5 \text{ lp}\cdot\text{mm}^{-1}$ (left), as shown in Figure S32. For a more precise assessment of spatial resolution, the modulation transfer function (MTF) of the scintillation screen was determined from the X-ray image of a slanted-edge (Figure S33). Spatial resolution is defined as the spatial frequency at which the MTF equals 20%. The SPA-mediated CsCu_2I_3 NWs exhibited a superior spatial resolution of $7.72 \text{ lp}\cdot\text{mm}^{-1}$, outperforming the commercial scintillator film of $\text{Gd}_2\text{O}_2\text{S:Tb}$ (GOS), which exhibited a spatial resolution of $6.20 \text{ lp}\cdot\text{mm}^{-1}$.

Consequently, the image resolution achieved with the CsCu_2I_3 NWs scintillator, which reached another critical parameter for scintillator, is the light yield, which reflects the X-ray-to-light conversion efficiency and serves as a metric for evaluating the detection capability of scintillator materials. The X-ray light yield of SPA-mediated CsCu_2I_3 NWs reached 77,500 photons per MeV, delivering an approximately ninefold enhancement, compared with W/O-mediated CsCu_2I_3 DCs (8,700 photons per MeV) (Figure S34). This value also surpassed commercially available BGO inorganic scintillator (8500 photons per MeV) and several conventional scintillators (Figure 5d and Table S10) [59–63], representing one of the highest light yields reported for perovskite NWs. This exceptionally high X-ray light yield is attributed to the multifunctional optimization effect of the SPA-mediated strategy, which comprehensively regulates multiple core parameters that govern scintillation performance. The physical origin of such performance improvement can be quantitatively explained by the classic scintillation light yield formula: $LY = 10^6 \cdot S \cdot Q / (\beta E_g)$, which takes into account the scintillator band gap (E_g), the transmission efficiency (S) of electron–hole pair energy to the luminescent center, and the intrinsic luminescence quantum efficiency (Q) [64, 65]. Besides, the parameter β denotes the average energy needed to create an electron–hole pair.

Distinctly, PLQY solely reflects the intrinsic radiative quantum efficiency (Q) under surface-limited UV excitation, while X-ray light yield is a full-scale comprehensive parameter dependent on both Q and S . SPA coordination simultaneously eliminates iodine vacancy defects to suppress carrier trapping loss, optimizes crystal microstructure to improve crystallinity, and reduces interfacial light scattering and self-absorption [66]. These synergistic optimizations contribute to the prominent enhancement in X-ray light yield.

To assess the dose response of SPA-mediated CsCu_2I_3 NWs, their RL intensity was measured at X-ray dose rates ranging from 0.02 to $33.12 \mu\text{Gy}_{\text{air}}\cdot\text{s}^{-1}$ (Figure S35). Figure S36 illustrates the integrated RL intensity of W/O-mediated CsCu_2I_3 DCs and SPA-mediated CsCu_2I_3 NWs as a function of incident X-ray dose rate, revealing an excellent linear relationship across this broad range, consistent with previous reports [27, 28, 34, 37]. The

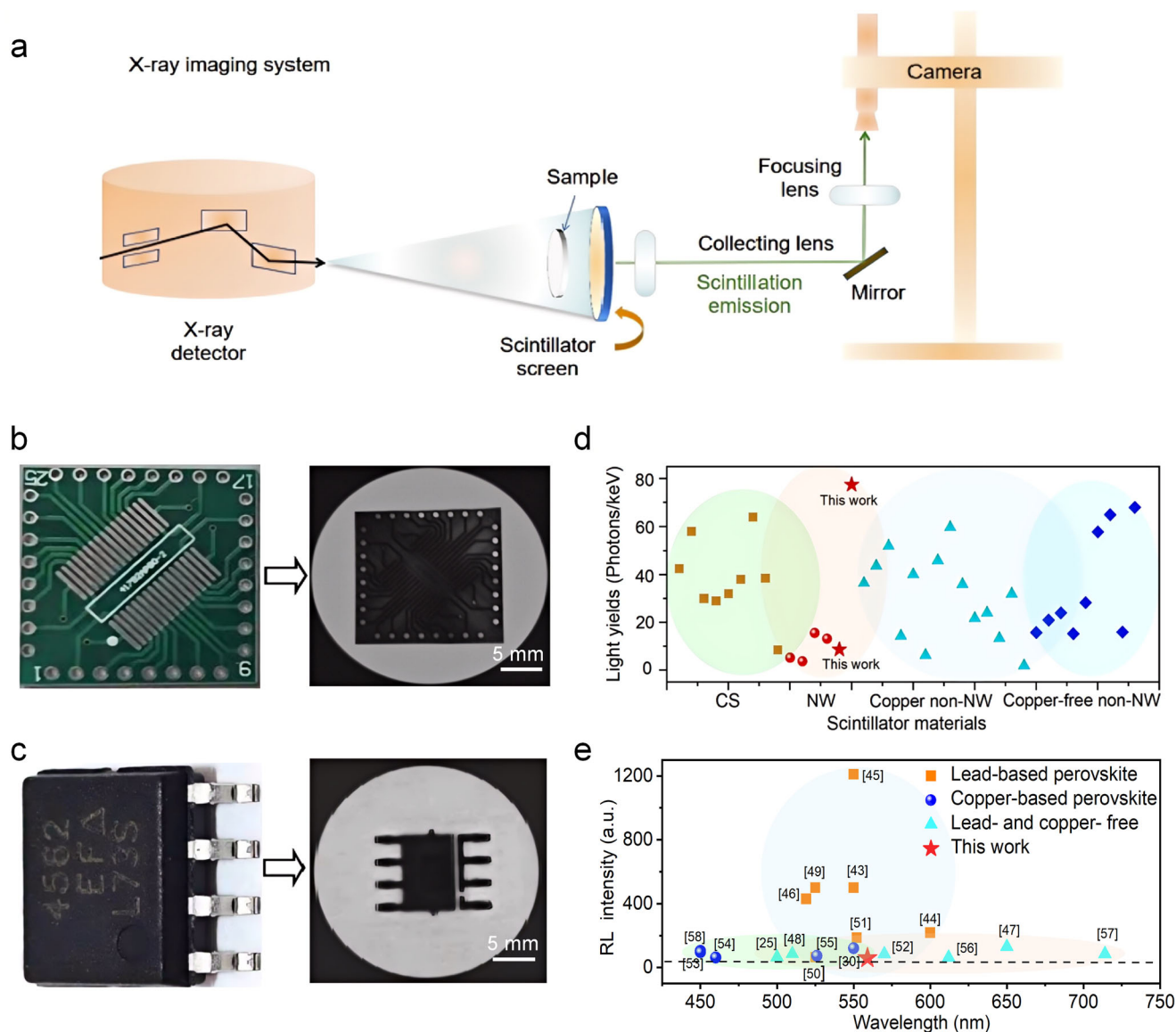


FIGURE 5 | Exploring the comprehensive applications and high-resolution X-ray imaging capabilities of CsCu₂I₃ NWs scintillators. (a) Schematic illustration of the X-ray imaging testing setup. (b,c) X-ray images of a semiconductor chip (2 × 2 cm) and a small electronic component: First row: Optical photographs recorded under daylight. Second row: X-ray images acquired using the CsCu₂I₃ NWs scintillator screen in our radiography setup (X-ray tube voltage: 50 kV; dose rate: 62.2 μGy_{air}·s^{−1}). (d) Comparison of light yields between CsCu₂I₃ NWs, commercial scintillators and several well-established scintillators. (e) Comparison of the lowest detection limit for different materials [25, 30, 43–58].

detection limit of the X-ray dose rate was determined to be 59.20 nGy_{air}·s^{−1} for SPA-mediated CsCu₂I₃ NWs (signal-to-noise ratio = 3), approximately 93 times lower than the dose rate required for standard X-ray medical diagnostics (5.50 μGy_{air}·s^{−1}) [67, 43]. Importantly, a comparison of the lowest detection limits for various materials is presented in Figure 5e. Collectively, these results demonstrate that CsCu₂I₃ is highly advantageous for achieving excellent X-ray image contrast. Considering the comprehensive performance of SPA-mediated CsCu₂I₃ NWs, including their outstanding scintillation properties, favorable physical characteristics suitable for practical implementation, and cost-effective advantages, these materials ultimately represent an ideal scintillator platform with significant potential for commercialization.

2.6 | Generality of the SPA Strategy

To verify the transferability of the SPA strategy beyond the prototype CsCu₂I₃ system, the identical ethanol-based SPA protocol has been implemented on two additional copper-halide systems with distinct structural dimensionalities and compositions. Cs₃Cu₂I₅ possesses a 0D electronic structure composed of isolated [Cu₂I₅]^{3−} units with blue STE emission, while Cu₂I₂[Dmphen]₂ represents a 0D molecular organic-inorganic hybrid copper iodide complex with red luminescence. When combined with 1D CsCu₂I₃ NWs, these three systems span dimensionalities from 1D to 0D and compositions from fully inorganic to organic-inorganic hybrid (Figure S37). Uniform luminescence enhancement is achieved for all three copper halide systems after identical SPA

treatment. Under UV illumination, SPA-modified CsCu_2I_3 (yellow emission), $\text{Cs}_3\text{Cu}_2\text{I}_5$ (blue emission), and $\text{Cu}_2\text{I}_2[\text{Dmphen}]_2$ (red emission) all exhibit markedly enhanced luminescence, compared with their untreated (W/O) reference samples. In precursor solution characterization, the SPA treatment converts the turbid and aggregated W/O dispersions into homogeneous, transparent, or uniformly colored solutions for all three systems, reflecting improved morphological homogeneity and suppressed aggregation-induced scattering. The SPA passivation mechanism relies on Lewis acid-base pairing between oxygen lone pairs of ethanol molecules and unsaturated surface Cu^+ centers; it therefore operates through the identical interfacial interaction pathway that takes effect regardless of crystal dimensionality or chemical composition. These multi-system experimental results demonstrate that the SPA strategy is not limited to CsCu_2I_3 but serves as a generalizable route to stabilize copper(I) halides and enhance the luminescence performance simultaneously.

3 | Conclusion

In summary, lead-free W/O- and SPAs-mediated CsCu_2I_3 scintillators have been successfully synthesized using an innovative LTC method at 0°C and atmospheric pressure. Moreover, the SPA framework establishes three mutually reinforcing protective layers within a single solvent additive: (i) a structural stabilization layer that arrests dissolution–redeposition shrinkage and preserves 1D morphological integrity during solvent removal; (ii) a redox stabilization layer that maintains a locally reducing microenvironment and suppresses $\text{Cu}^+ \rightarrow \text{Cu}^{2+}$ oxidation across all three crystallization stages; and (iii) an interfacial coordination stabilization layer in which the alcohol O–H groups form weak coordination bonds with under-coordinated surface Cu^+ sites, reconstructing and passivating defect centres at the atomic level. Different from conventional solvent engineering and post-synthesis surface passivation approaches that only optimize single performance dimension, our one-step SPA-mediated LTC strategy innovatively regulates the liquid–solid transition stage, simultaneously mitigating lattice strain, eliminating surface Cu^+ oxidation defects and suppressing nonradiative recombination, which realizes comprehensive performance promotion unavailable in prior studies. Demonstrated on CsCu_2I_3 as a model 1D Cu–I scintillator, ethanol-mediated SPA treatment raises PLQY from 12.78% to 21.65%, increases X-ray light yield approximately ninefold to 77,500 photons MeV^{-1} , also approximately ninefold higher than commercial available BGO inorganic scintillator. Additionally, these ethanol-mediated CsCu_2I_3 NWs demonstrate remarkable performance with a detection limit of 59.20 $\text{nGy}_{\text{air}} \cdot \text{s}^{-1}$, a spatial resolution of 7.72 $\text{lp} \cdot \text{mm}^{-1}$, excellent X-ray imaging capabilities, and long-term operating stability. Beyond the high-performance CsCu_2I_3 system, identical SPA treatment achieves consistent luminescence enhancement on representative 0D hybrid copper iodide and 3D $\text{Cs}_3\text{Cu}_2\text{I}_5$ scintillators, fully verifying the generalizable nature of the proposed ligand engineering framework for diverse copper halide materials. Overall, this straightforward SPA-mediated CsCu_2I_3 NWs growth strategy assisted by surface molecule coordination offers a facile and effective pathway for preparing high-quality, nontoxic copper-iodide-based NWs, which can be extended to other halide perovskites and nanomaterials. These advancements pave the way for broader applications in various fields, including LED

emitters or phosphors, X-ray images, real-time X-ray detectors, other related nanowire-based optoelectronic devices and even energy applications.

Acknowledgments

This work was financially supported by the Heilongjiang Provincial Natural Science Foundation of China (No. LH2024A022), Daqing Leading Talent Qingyan Program of New Yan Special Project (No. DQXY202506), the National Natural Science Foundation of China (Nos. 62404104, 21827812, 21890741), and the Natural Science Foundation of Jiangsu Province (No. BK20241465). The authors gratefully acknowledge the support of the Vacuum Interconnect Nano X Research Facility (NANO-X) at the Suzhou Institute of Nano-Tech and Nano-Bionics, and Chinese Academy of Sciences and thank beamlines BL03HB and BL14B1 at the Shanghai Synchrotron Radiation Facility (SSRF) for providing beam time.

Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

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Supporting Information

Additional supporting information can be found online in the Supporting Information section.

Supporting File: agt270420-sup-0001-SuppMat.docx.