Ligand Modified Cesium Lead Bromide for X-ray Scintillators

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Abstract—Perovskite of CsPbBr₃ nanocrystals show enhanced stability after organic ligand passivation while maintaining scintillation efficiency, which has been verified by theoretical calculations and experimental results. In this work, ligand modified CsPbBr₃ scintillators demonstrate exceptional performance for radiation detection, exhibiting a low detection limit of 49.2 nGy/s and <40 ns decay time. These properties, combined with cost-effective fabrication and spectral compatibility with Si detectors, position CsPbBr₃ as a promising alternative to conventional scintillators in X-ray imaging applications.

Keywords—perovskite, CsPbBr3, scintillator, Ligand modification

I. INTRODUCTION

X-ray detectors and their imaging systems have become indispensable components in medical imaging, industrial nondestructive testing, and aerospace applications[1]. For the core component of X-ray scintillators, the critical factors determining their operational performance lie in the selection of photoelectric conversion materials and the design of device architectures[2]. Currently, commercial scintillator materials such as CdWO₄ and CsI face limitations in widespread applications due to their inherent constraints: their constituent elements possess relatively low atomic numbers, resulting in inadequate X-ray absorption coefficients, susceptibility to radiation damage, and high manufacturing costs[3].

In recent years, a new generation of semiconductors represented by perovskite-type metal halides with ABC3 structures (A = organic/inorganic cations, B = metal cations, C = halide anions $Cl^{-}/Br^{-}/I^{-}$) has been extensively applied in optoelectronics[4]. These metal halides demonstrate advantages including tunable emission spectra and high luminescence efficiency, while achieving dimensional control (3/2/1/0 electronic dimension) through compositional engineering[5]. Their strong X-ray absorption capability, long carrier diffusion length, and low fabrication costs have attracted significant global research attention[6]. Among them, CsPbBr₃ currently stands as the most intensively investigated perovskite. As early as 2018, researchers employed CsPbBr₃ in low-dose X-ray scintillator detection and imaging, achieving a spatial resolution of 5 lp/mm, though compromised by inherent instability[7]. Subsequent studies proposed constructing CsPbBr₃ systems to enhance stability while improving detection performance for X-ray imaging, yet the stability improvement remained limited. These findings underscore that enhancing the stability of metal halide perovskites constitutes the primary challenge for developing high-performance X-ray detectors. This work presents a ligand modification strategy to simultaneously improve the stability and photoluminescence efficiency of CsPbBr₃ nanocrystals for X-ray scintillator applications.





Fig. 1 Calculated (a) attenuation coefficients, and (attenuation efficiency) of CsPbBr₃, CdWO4, and CsI at different X-ray energies

As shown in Figure 1a, we began by calculating the absorption spectrum for perovskite (CsPbBr₃) and traditional semiconductors (CdWO₄ and CsI) over a broad range of photon energies (from 1 to 100 keV) using the photon cross-section database. CsPbBr₃ exhibits comparable X-ray attenuation coefficients to commercial scintillators, attributed to its high average atomic number (Z = 48.4). Under typical medical imaging X-ray energies (e.g., 20 keV), CsPbBr₃ demonstrates superior X-ray absorption efficiency compared to conventional scintillators like CdWO₄ (Z = 25.67) and CsI (Z = 54) at equivalent thicknesses (Fig. 1b). The relationship between attenuation coefficient and atomic number is[8]:

$$\mu/\rho \propto Z^4/E^3 \tag{1}$$

where μ/ρ is the mass attenuation coefficient, Z is the average atomic numbers, and E is the X-ray energy. This significant performance advantage, combined with its solution-processable characteristics, positions CsPbBr₃ as a promising candidate for next-generation X-ray scintillators.



Fig. 3 (a) Relaxed surface models for simulating the adsorption of OA/DA molecules on the $CsPbBr_3$ surface. The insets are the zoomed-in plot of the bonded regions. (a) OA on top of the pristine CsBr-terminated surface. (b) DA on top of the pristine CsBr-terminated surface. (c) OA bonding with a Br-vacancy. (d) DA bonding with a Br-vacancy. (e) The binding energies of the four interfaces

Figure 3a-d presents the surface models employed to simulate the adsorption of oleic acid (OA)/2-Hexidodecanoic acid (DA) on the CsPbBr3 surface. To eliminate artificial interactions between molecules and periodic images of the model, large vacuum regions (>15 Å) were introduced in both in-plane and out-of-plane directions. The bottom CsPbBr₃ layer was fixed at their bulk structural parameters, while the upper two CsPbBr₃ layers were fully relaxed to account for surface reconstruction effects and bonding interactions with adsorbates. Structural relaxation was meticulously performed using convergence criteria of 0.01 eV/Å for residual forces and 10⁻⁶ eV for energy, as the numerical convergence sensitivity could critically influence the validity of calculated binding energies. Since numerical convergence sensitivity could critically affect the reliability of binding energy calculations, the structural relaxation was meticulously executed. Figure 3e illustrates the OA/DA binding strengths to CsPbBr3 for four distinct adsorption models, revealing that DA exhibits stronger binding affinity than OA. We also investigated OA/DA adsorption on the pristine CsBr-terminated surface (Figs. 3a-b), which represents the most prevalent termination surface in CsPbBr₃ nanocrystals. The hydrogen atoms from the -COOH groups were initially positioned atop Br anions, as small molecules are generally hypothesized to bind to CsBr surfaces via hydrogenbonding interactions. In addition, as shown in Figure 3e, the binding of DA ligand to CsPbBr3 nanocrystals is clearly more stable than that of OA ligand, with $\Delta E = 0.202 \text{ eV}$.

To evaluate the imaging performance of the X-ray scintillators, the object to be tested was positioned between the X-ray source and scintillator, where its material-dependent X-ray attenuation properties generated spatially modulated radiation patterns. As shown in Figure 4a, the scintillator converted these varying X-ray intensities into corresponding visible light emissions, which were subsequently captured by a commercial camera. The resulting electrical signals from the camera were then processed for digital image reconstruction and display. As shown in Figure 4b, as-synthesized CsPbBr₃-DA scintillator presents a low detection limit of 49.2 nGy/s, and a short response time (rise time: 1.2 ns, fall time: 35.3).



Fig. 4 (a) Schematic diagram of scintillator imaging and its imaging of chips. (b) Detection limit. (c) Response time

III. CONCLUSION

Simulation calculations and experiments have shown that ligand modified CsPbBr₃ scintillators demonstrate enhanced stability and exceptional performance for X-ray, exhibiting a low detection limit of 49.2 nGy/s and <40 ns decay time. Owing to the aforementioned superior optoelectronic properties, CsPbBr₃ is positioned as a promising candidate for broad applications in X-ray detection and imaging technologies.

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