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▪ **Research Interests:** Nanomaterials, Perovskites, MXenes, Photovoltaic-Devices (Solar cells, Photodetectors), & Their Biological (Multimodal Bacteria killing, Cancer, DNA-oxidation, Imaging) & some 'off the shelf' applications like (Novel Radiation detection & Photovoltaics for space).



Education

Aug 2023 onwards	PhD 3 rd year [Under Prof. Sayan Bhattacharyya]
July 2022 onwards	Prime Ministers Research Fellowship
2019 onwards	Integrated PhD Chemistry, (MS completed in June 2022 with 8.75 CGPA)
2016-2019:	BSc. Industrial Chemistry, University of Delhi, 1 st Division -77.44% (College Rank-3 rd)
2016:	Class 12 th , CBSE Board, 1 st Division - 88.8% (School Rank- 2 nd)
2014:	Class 10 th , ICSE Board, 1 st Division - 88% (District Rank-2 nd)

Awards, Scholarships & Achievements:

2023:	Training of GC-MS for Photocatalytic CO ₂ reduction Studies
	Training of AFM Instrument handling for measurements like(AFM[Contact/Tapping], KPFM, EFM, PFM, c-AFM, Liquid AFM, STM & electro-chemical AFM)
	Training of SCXRD instrument handling
	Fabrication of Photodetector and Solar Cells

Participation in APMD-2023 conference by S&T Digital (Chaired by **Prof. Satish Ogale**)
Workshop & Training of NMR & MNova software
TAship of course Molecules of life @Deshbandhu College (University of Delhi)
TAship of Solar Photovoltaics Course @ NPTEL by **Prof. Ashish Garg** (IIT Kanpur)
Participation and Best Question Award in ViPerCon-2023 (by **Prof. Michael Saliba**)
Student Membership of PRSI (Perovskite Research Society of India)
Student Membership of ACS (American Chemical Society)
Certification Short Term Course on MXene Synthesis, Characterization, Processing and electrochemistry organized by A J Drexel Institute (Supervised by **Prof. Yury Gogotsi**)
2022: Prime Ministers Research Fellow (Id: 0501975)
Qualified TOEFL (Score: 84)
TAship of CH5103 (Supramolecular Chemistry and Applications)
Qualified GATE

- 2021:** Online Short-Term Training on X-ray Diffraction Theory (6th Sep 2021 - 15th Sep 2021) organized by MNNIT Bhopal
Virtual Online Conference on Multifunctional advanced materials
CSIR-CECRI Skill Training & Development Program (AIR-3)
Participation in AWSAR, DST
- 2020:** Nano-ge conference participation
- 2019:** Brainiac All University Chemistry Quiz (DBC, DU Rank-3rd)
Qualified Joint Admission (JAM-2019) Test for M.Sc. admission
BSc. Industrial Chemistry, (College Rank- 3rd)
Qualified CSIR-NET (Lectureship Qualification Examination in Chemical Science for the all-Indian Universities)

Professional Development:

- Synthesis of Perovskites (Bulk, Nano & Single Crystals)
- Characterizations & Analysis (UV, PL, SEM, TEM, AFM, PXRD, SCXRD, Raman, FTIR, TGA/DSC, CD, NMR, Mass)
- Instrument Handling (UV, PL, SCXRD, TGA-FTIR, AFM/KPFM/PFM)
- Softwares Nova/WSXM (For AFM analysis), Gatan (For TEM analysis), GSAS (For Rietveld analysis), Imagej (For SEM analysis), Fityk (For XPS analysis), Origin (For graph plotting: UV, PL, TCSPC, Raman etc.), Chemdraw (For making structures), MS office

Publications:

1. Kumari Raksha,# Noufal Kandoth,#* **Shresth Gupta**, Subhadeep Gupta, Sumit K. Pramanik, Amitava Das*. Modulating Resonance Energy Transfer with Supramolecular Control in Layered Hybrid Perovskite and Chromium Photosensitizer Assembly. *ACS Appl. Mater. Interfaces* **2023**, 15, 21, 25148–25160
2. Arnab Mandal, Samrat Roy, Anamika Mondal, **Shresth Gupta**, Bipul Pal, Sayan Bhattacharyya *. Ambient-Stable Near Unity Photoluminescence Quantum Yield in Two-dimensional Tin Bromide Perovskites. *J. Phys. Chem. Lett.* **2022**, 13, 39, 9103–9113
3. Noufal Kandoth,* Sonu Pratap Chaudhary, Subhadeep Gupta, Kumari Raksha, Atin Chatterjee, **Shresth Gupta**, Safakath Karuthedath, Catherine S. P. De Castro, Frédéric Laquai, Sumit K. Pramanik, Sayan Bhattacharyya,* Amirul I. Mallick,* Amitava Das*. Multimodal Biofilm Inactivation Using a Photocatalytic Bismuth Perovskite-TiO₂ based Hybrid with M-scheme Heterojunctions. *ACS Nano*, **2023**, 17, 10393-10406
4. Arnab Mandal, **Shresth Gupta**, Supriti Dutta, Swapan K. Pati, Sayan Bhattacharyya * Transition from Dion Jacobson Hybrid Layered Double Perovskites to 1D Perovskites for Ultraviolet to Visible Photodetection. *Chem. Sci.*, **2023**, 14, 9770-9779

Ongoing Works:

5. Noufal Kandoth, † * **Shresth Gupta**, † Kumari Raksha, Subhadeep Gupta, Sonu Pratap Chaudhary, Amir ul Islam, * Sayan Bhattacharyya, * Amitava Das. * Nanoparticulate Hybrid Metal Halide Perovskite for Multi-modal Gram-Negative Bacterial/Biofilm inactivation via selective , photocatalytic amplification of nitric oxide and hydroxyl radical ion generation. (**Manuscript Submitted**)

6. **Shresth Gupta**, Sema Sarisozen, Sanjua Khuntia, Priya Mahadevan, Felix Lang, Sayan Bhattacharyya. * Structure-Property relationship in Bi/Sb based Low-Dimensional Organic Inorganic Hybrid Iodides for X-ray Detection. (**Manuscript Under Preparation**)

7. **Shresth Gupta**, † Sitavro Mandal, † Anamika Mondal, Sema Sarisozen, Sayan Bhattacharyya*. Dimensional Engineering in Hybrid Layered Double Perovskites for Photo and X-ray detection. (**Manuscript Under Preparation**)

8. Anamika Mondal, **Shresth Gupta**, Sayan Bhattacharyya. * Reconfiguring the organic inorganic hybrid polyhedra to boost the charge carrier density and mobility. (**Manuscript Under Preparation**)

Referees:

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- **Prof. Amitava Das, Dean of Faculty Affairs, IISER Kolkata, Dept. of Chemical Sciences, Mo. No: 9428051283, Email: Amitava@iiserkol.ac.in**
- **Prof. Rahul Banerjee, IISER Kolkata, Dept. of Chemical Sciences, Mo. No: 6297976236, Email: r.banerjee@iiserkol.ac.in**

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- Birth Date: 31 August 1999
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Spacer Switched Two-Dimensional Tin Bromide Perovskites Leading to Ambient-Stable Near-Unity Photoluminescence Quantum Yield

Arnab Mandal, Samrat Roy, Anamika Mondal, Shresth Gupta, Bipul Pal, and Sayan Bhattacharyya*



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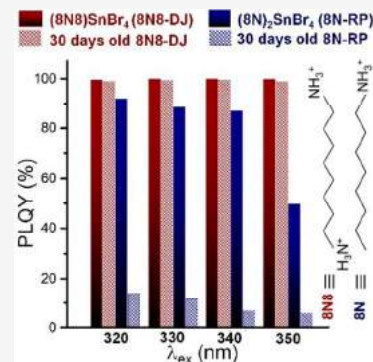


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ABSTRACT: Semiconductor nanostructures with near-unity photoluminescence quantum yields (PLQYs) are imperative for light-emitting diodes and display devices. A PLQY of $99.7 \pm 0.3\%$ has been obtained by stabilizing 91% Sn^{2+} in the Dion–Jacobson (8N8)SnBr₄ (8N8-DJ) perovskite with 1,8-diaminooctane (8N8) spacer. The PLQY is favored by a longer spacer molecule and out-of-plane octahedral tilting. The PLQY shows one-month ambient stability under high relative humidity (RH) and temperature. With *n*-octylamine (8N) spacer, Ruddlesden–Popper (8N)₂SnBr₄ (8N-RP) also shows PLQY of $91.7 \pm 0.6\%$, but it has poor ambient stability. The 5–300 K PL experiments decipher the self-trapped excitons (STEs) where the self-trapping depth is 25.6 ± 0.4 meV below the conduction band because of strong carrier–phonon coupling. The microsecond long-lived STE dominates over the band edge (BE) peaks at lower excitation wavelengths and higher temperatures. The higher PLQY and stability of 8N8-DJ are due to the stronger interaction between SnBr₆⁴⁻ octahedra and 8N8 spacer, leading to a rigid structure.



Metal halide perovskites are a disruptive class of materials because of their potential application in optoelectronics and photovoltaics,^{1–4} particularly so when they are prepared with minimal structural disorder, high thermal resistance, and photostability. Solution-processed all-inorganic CsPbX₃ (X = Cl, Br, I) nanocrystals (NCs) have reached 100% PLQY because of the synthetic marvels that resulted in a substantial reduction of the nonradiative recombination centers and trap-mediated nonradiative losses.⁵ Such a high PLQY can be sustained by maintaining the phase stability of these NCs under ambient conditions, which is an arduous task. Two-dimensional (2D) perovskites have emerged as next-generation systems with better moisture and heat stability.⁶ Among them, the Ruddlesden–Popper (RP) and Dion–Jacobson (DJ) phases are most common, denoted by the formula A'₂A_{n-1}M_nX_{3n+1} and A''A_{n-1}M_nX_{3n+1}, respectively, where A' is a monovalent and A'' is a bivalent interlayer spacer cation; A is a smaller monovalent cation (MA⁺, FA⁺, or Cs⁺); M is a divalent metal (Pb²⁺ or Sn²⁺); and X is Cl⁻, Br⁻, or I⁻. The A' and A'' hydrophobic alkyl ammonium chains render stability to the 2D perovskites and act as a barrier between the MX₆⁴⁻ octahedral layers forming a quantum well-like structure by increasing the potential barrier. Blessed with a strong quantum confinement by the bulky spacer cations, RP and DJ perovskites have shown decent PLQY.^{7–10} However, a gap persists since the ambient stability of PLQY is rarely explored or the origin of PL emission is seldom explained in Sn-based 2D perovskites. The PL stability can be rendered by B-site doping,¹⁰ using modified RP structures,¹¹ by antisolvent processing, etc.¹²

The RP phase, PEA₂Cs_{2.4}MA_{0.6}Pb₄Br₁₃ (PEA: phenylethylammonium; MA: methylammonium), capped with triphenylphosphine oxide has demonstrated 97% PLQY.⁷ The Pb-free RP perovskites such as (C₁₈H₃₅NH₃)₂SnBr₄ and (C₈H₁₇NH₃)₂SnBr₄ have 88 and 98% PLQY, respectively.^{8,9} There are only a few DJ perovskites with appreciable PL emission; the 88% quantum yield in ODASnBr₄ (ODA: protonated 1,8-octanediamine) is a rare observation.¹³ The RP and DJ phases offer the advantages of a tunable electronic structure depending on the number of layers (*n*),¹⁴ decent luminescence by the confinement of excitons within the potential barrier,¹⁵ and stabilization of the labile oxidation states by the hydrophobic organic spacer.¹⁶ However, the RP phases lack potential for use in optoelectronics because of the insulating gap between two layers of the protonated ligands held together by van der Waals interactions.¹⁷ The DJ perovskites benefit from the H-bonding between the divalent organic cation and the inorganic perovskite octahedra at both ends, thereby rendering better structural stability¹⁸ and resulting in potential use in optoelectronic devices.^{19,20}

On the basis of this logic, we have changed the interlayer ammonium spacer from *n*-octylamine (8N) to 1,8-diaminooctane (8N8) to synthesize (8N)₂SnBr₄ (8N-RP) with PLQY of

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Modulating Resonance Energy Transfer with Supramolecular Control in a Layered Hybrid Perovskite and Chromium Photosensitizer Assembly

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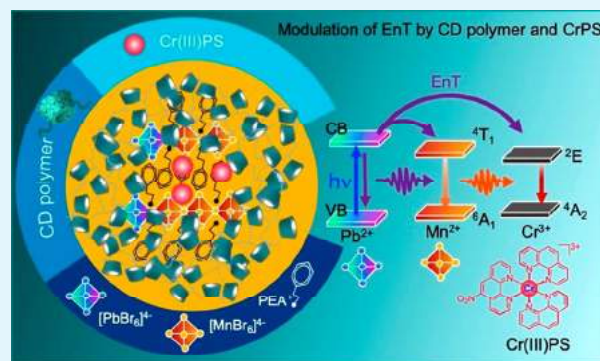
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ABSTRACT: Recently, the low-dimensional organic–inorganic halide perovskites (OIHP) have been exploited heavily for their favorable exciton dynamics, broad-band emission, remarkable stability, and tunable band-edge excited-state energy compared to their 3D counterparts for potential optoelectronic applications. Low-dimensional perovskites are generally good candidates for utilization as room-temperature photoluminescence (PL) materials. Further, doping divalent transition metals like Mn^{2+} into OIHP is expected to introduce a ${}^4\text{T}_1$ – ${}^6\text{A}_1$ -based low-energy luminescence emission around 600 nm; an optical property that is favorable for biomedical optoelectronics. Doping Mn^{2+} in the perovskite lattice is also expected to induce the generation of cytotoxic singlet oxygen species (${}^1\text{O}_2$), a ROS that is being exploited for various therapeutic applications. To integrate these optical and therapeutic properties of a 2D $(\text{PEA})_2\text{PbBr}_4$ (Pb PeV; PEA = phenylethylammonium cation) perovskite alloyed with Mn^{2+} ions (Mn:PbPeV) and the option for a photoinduced energy transfer process involving a Cr(III)-based ${}^1\text{O}_2$ generating photosensitizer (CrPS), we designed a unique purpose-built nanoassembly (Mn:PbPeV@PCD) using the encapsulation properties of a water-soluble polymer derived from β -cyclodextrin (PCD). Here the PCD is observed to modulate the classical internal energy transfer of Pb^{2+} exciton to alloyed Mn^{2+} orange emission, resulting in the emergence of a new blue emission. The addition of CrPS into the Mn:PbPeV@PCD to generate the CrPS@Mn:PbPeV@PCD assembly results in restoring perovskite luminescence followed by the external energy transfer to CrPS. We have elucidated the mechanism of these cascade energy transfer processes between multiple components using steady-state and time-resolved luminescence techniques. Efficient ROS generation and its potential to induce an oxidation reaction of a biomolecule are realized using guanine as the target molecule. Further photoinduced cleavage studies with biomolecules confirmed the efficacy of the nanoassembly in inducing the cleavage of guanine-rich DNA. The study opens up a new direction in the field of perovskite for biomedical applications.

KEYWORDS: 2D hybrid organic–inorganic perovskite, cyclodextrin polymer, chromium photosensitizer, energy transfer, photo-oxidation



INTRODUCTION

Metal halide perovskite-based materials have been studied extensively in the past decade because of their unique optoelectronic properties and the option to fine-tune such properties through modulation of their crystalline band edges for various advanced applications.^{1–4} In low-dimensional OIHPs, charge carriers typically couple to a soft lattice and result in self-trapped excitons, which attributes to a broadband emission and room-temperature photoluminescence (PL).⁵ The OIHPs also garnered an upsurge of scientific interest over their bulk 3D counterparts for improved photoemission, moisture resistance, and thermostability.^{6–8} Further, doping of the divalent transition metal ions, like Ni^{2+} , Bi^{3+} , and Mn^{2+} , in the B-site of 2D-based perovskites is known to facilitate a broad-band orange-red emission from the ${}^4\text{T}_1$ – ${}^6\text{A}_1$ transition.

Such emission processes typically possess a fairly long emission decay lifetime in the millisecond time range.^{9–11} Among different transition metal ions, doping of Mn^{2+} into the crystal lattice of two-dimensional (2D) layered lead halide perovskites with the formula A_2PbX_4 (A = organic cation, X = halide) leads to the sharing of each corner of $[\text{PbBr}_6]^{4-}$ octahedra to form isotropic inorganic layer networks that are separated from each other by A-site organic cation layers.^{12,13} Each adjacent layer is

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Transition from Dion–Jacobson hybrid layered double perovskites to 1D perovskites for ultraviolet to visible photodetection†

Arnab Mandal,^a Shresth Gupta,^a Supriti Dutta,^b Swapan K. Pati^b and Sayan Bhattacharyya^b

New perovskite phases having diverse optoelectronic properties are the need of the hour. We present five variations of $R_2AgM(III)X_8$, where $R = NH_3C_4H_8NH_3$ (4N4) or $NH_3C_6H_{12}NH_3$ (6N6); $M(III) = Bi^{3+}$ or Sb^{3+} ; and $X = Br^-$ or I^- , by tuning the composition of $(4N4)_2AgBiBr_8$, a structurally rich hybrid layered double perovskite (HLDP). $(4N4)_2AgBiBr_8$, $(4N4)_2AgSbBr_8$, and $(6N6)_2AgBiBr_8$ crystallize as Dion–Jacobson (DJ) HLDPs, whereas 1D $(6N6)SbBr_5$, $(4N4)BiI$ and $(4N4)SbI$ have *trans*-connected chains by corner-shared octahedra. Ag^+ stays out of the 1D lattice either when $SbBr_6^{3-}$ distortion is high or if Ag^+ needs to octahedrally coordinate with I^- . Band structure calculations show a direct bandgap for all the bromide phases except $(6N6)_2AgBiBr_8$. $(4N4)_2AgBiBr_8$ with lower octahedral tilt shows a maximum UV responsivity of $18.8 \pm 0.2 \text{ A W}^{-1}$ and external quantum efficiency (EQE) of $6360 \pm 58\%$, at 2.5 V. When self-powered (0 V), $(4N4)SbI$ has the best responsivity of $11.7 \pm 0.2 \text{ mA W}^{-1}$ under 485 nm visible light, with fast photoresponse ≤ 100 ms.

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Introduction

In the search for next-generation photoabsorbers for optoelectronics and photovoltaics, halide perovskites have garnered maximum interest, owing to the unwavering discovery of new phases with varying dimensionalities.^{1,2} Slowly but steadily, the shift in focus has been towards lead-free systems having improved moisture and thermodynamic stabilities, but with an out-of-the-common lead-perovskite-like defect tolerance.³ In this context, double perovskites with a general formula $A_2M(I)M(III)X_6$ [Pb^{2+} replaced by the combination of monovalent, $M(I)$, and trivalent, $M(III)$, cations, $A =$ methyl ammonium (MA^+), formamidinium (FA^+) and/or Cs^+ , and $X = Cl^-$, Br^- or I^-] are more benign having better stability. More than 100 double perovskites having an assorted combination of A , $M(I)$, $M(III)$ and X were predicted to be thermodynamically stable in terms

of their structural tolerance and octahedral factor.^{4,5} Among them, $Cs_2AgBiBr_6$ has established itself as a benchmark lead-free double perovskite due to its similar 3D structure to Pb-containing systems, along with high carrier mobility and lifetime, low effective carrier mass, and thermodynamic stability.^{6,7} Nevertheless, because of the contributions of Ag^+ and Bi^{3+} orbitals at the band edge position, $Cs_2AgBiBr_6$ has an indirect bandgap which limits its optoelectronic applications.⁴

An indirect to direct bandgap transition can be made possible by the dimensional reduction of 3D double perovskites to generate HLDPs.⁸ The 2D modification is achieved by introducing bulky monoammonium or diammonium cations between inorganic layers, especially for a single-layered inorganic framework ($n = 1$), where a direct bandgap results from the contribution of single metal orbitals to the valence band maxima (VBM; Bi p-orbital) and conduction band minima (CBM; Ag d-orbital) of double perovskites.⁹ To date, about 40 HLDPs have been synthesized with various compositions of $M(I)$ and $M(III)$, and among them, $(BA)_4AgBiBr_8$ and $(BA)_2CsAgBiBr_7$ ($BA =$ butyl ammonium cation) are the first reported HLDP structures with $n = 1$ and 2, having direct and indirect bandgaps, respectively.⁹ Most of them exist in the Ruddlesden–Popper (RP) phase and a few adopt the DJ structure. RP and DJ phases have the generalized formulae $A'_2A_{n-1}M_nX_{3n+1}$ and $A''A_{n-1}M_nX_{3n+1}$, respectively, where A' is monovalent and A'' is a bivalent bulky organic spacer cation, A is a smaller monovalent cation, M is a divalent metal or a combination of monovalent and trivalent metals, n is the number of inorganic layers and X is the halide. Accompanied by strong hydrogen bonding between the

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† Electronic supplementary information (ESI) available: Simulated XRD patterns; FESEM images; EDAX spectra; XPS plots; electronic band structure without SOC for HLDPs and 1D perovskites; light intensity dependent $J-V$ and EQE plots; potential dependent EQE and detectivity plots; chronoamperometry plots; photodetector data; comparison tables of HLDP and 1D perovskite photodetectors; Nyquist plot; Bode plot; stability plot; self-powered photodetector data. CCDC 2256088–2256091. For ESI and crystallographic data in CIF or other electronic format see DOI: <https://doi.org/10.1039/d3sc01919e>



Multimodal Biofilm Inactivation Using a Photocatalytic Bismuth Perovskite–TiO₂–Ru(II)polypyridyl-Based Multisite Heterojunction

Noufal Kandoth,^{*,†} Sonu Pratap Chaudhary,[†] Subhadeep Gupta, Kumari Raksha, Atin Chatterjee, Shresth Gupta, Safakath Karuthedath, Catherine S. P. De Castro, Frédéric Laquai, Sumit Kumar Pramanik, Sayan Bhattacharyya,^{*} Amirul Islam Mallick,^{*} and Amitava Das^{*}



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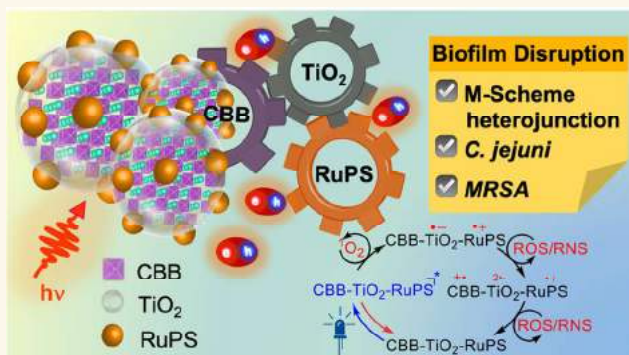
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ABSTRACT: Infectious bacterial biofilms are recalcitrant to most antibiotics compared to their planktonic version, and the lack of appropriate therapeutic strategies for mitigating them poses a serious threat to clinical treatment. A ternary heterojunction material derived from a Bi-based perovskite–TiO₂ hybrid and a [Ru(2,2'-bpy)₂(4,4'-dicarboxy-2,2'-bpy)]²⁺ (2,2'-bpy, 2,2'-bipyridyl) as a photosensitizer (RuPS) is developed. This hybrid material is found to be capable of generating reactive oxygen species (ROS)/reactive nitrogen species (RNS) upon solar light irradiation. The aligned band edges and effective exciton dynamics between multisite heterojunctions are established by steady-state/time-resolved optical and other spectroscopic studies. Proposed mechanistic pathways for the photocatalytic generation of ROS/RNS are rationalized based on a cascade-redox processes arising from three catalytic centers. These ROS/RNS are utilized to demonstrate a proof-of-concept in treating two elusive bacterial biofilms while maintaining a high level of biocompatibility (IC₅₀ > 1 mg/mL). The *in situ* generation of radical species (ROS/RNS) upon photoirradiation is established with EPR spectroscopic measurements and colorimetric assays. Experimental results showed improved efficacy toward biofilm inactivation of the ternary heterojunction material as compared to their individual/binary counterparts under solar light irradiation. The multisite heterojunction formation helped with better exciton delocalization for an efficient catalytic biofilm inactivation. This was rationalized based on the favorable exciton dissociation followed by the onset of multiple oxidation and reduction sites in the ternary heterojunction. This together with exceptional photoelectric features of lead-free halide perovskites outlines a proof-of-principle demonstration in biomedical optoelectronics addressing multimodal antibiofilm/antimicrobial modality.

KEYWORDS: bismuth perovskite halides, multiheterojunction, TiO₂, ruthenium polypyridyl complex, bacterial biofilm



INTRODUCTION

The global emergence of antibiotic-resistant biofilms and associated antimicrobial drug resistance (AMR) calls for the exploration of efficient methods and cross-disciplinary therapeutic interventions. A recent study provides the most comprehensive assessment of the global AMR as the leading cause of death around the world.^{1–3} This demands an intersectoral response to address therapeutic challenge, especially after the postpandemic changes in the healthcare landscape.^{4,5} A fresh approach beyond archetypical resistance-prone molecular antibiotic analogues is needed in this regard.⁶

Recently, antimicrobial nanosystems have garnered an upsurge of research interest against microbial infections by virtue of tuning their physicochemical properties and polyvalent

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