Optical and Charge Transport Properties of Halide Perovskite Nanocrystals for Multifunctional Devices

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- NNETRA, INUP (Meity)
- DST- ANRF, Nanomission

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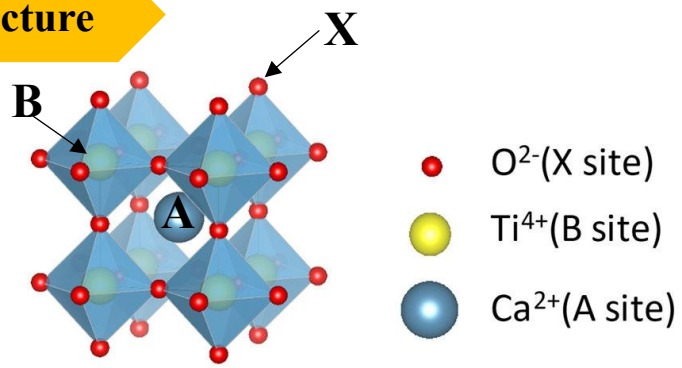
Halide Perovskites

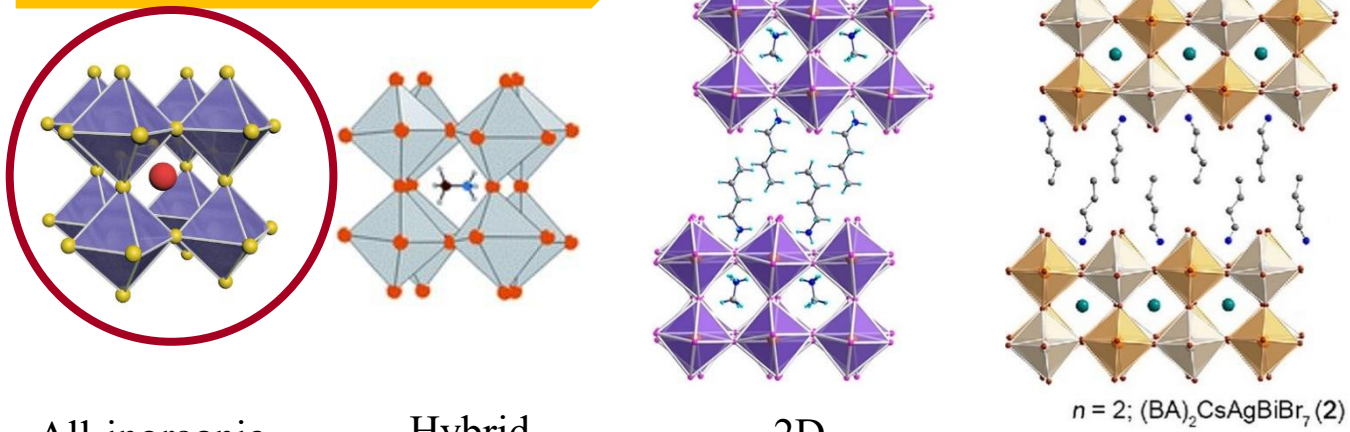
Structure



General form of perovskites: $\mathbf{ABX_3}$

A = Cs^+, MA^+, FA^+
B = Pb^{2+} , Sn^{2+}, etc.
X = Cl^-, Br^-, I^-

Different types of perovskites



All-inorganic perovskite | Hybrid perovskite | 2D perovskite | Double perovskite

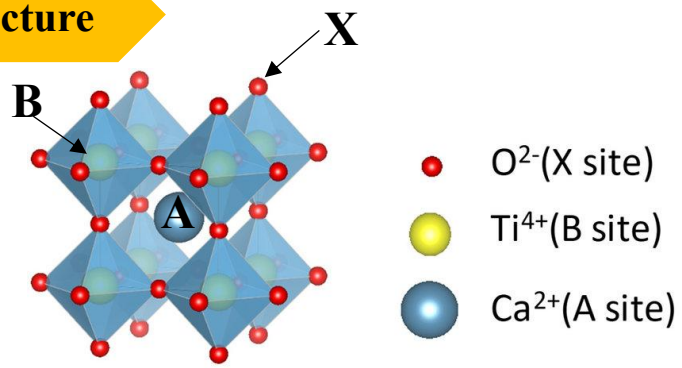
ACS Energy Lett. 2021, 6, 8, 2750–2754

Phases of perovskites

Cubic (α) | Tetragonal (β) | Orthorhombic (γ) | Non-perovskite (δ)

Halide Perovskites

Structure



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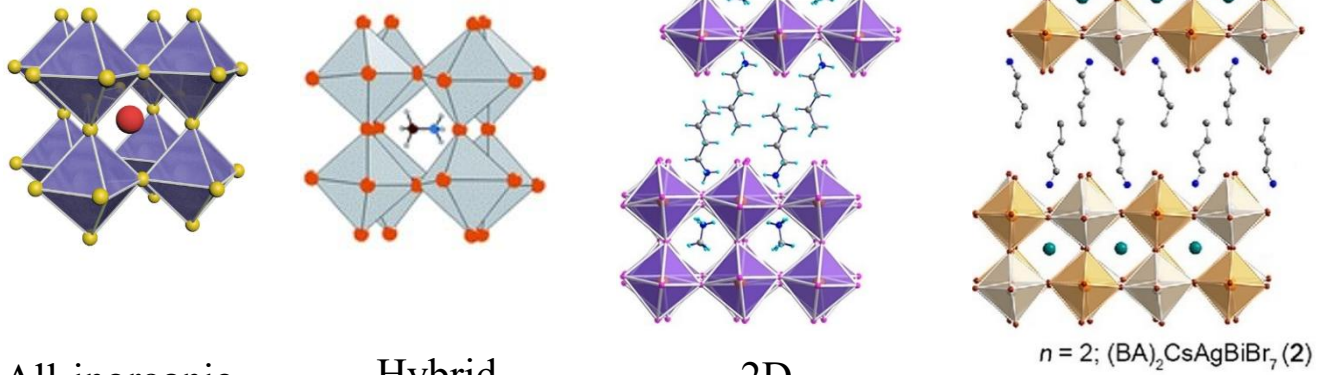

All-inorganic perovskite | Hybrid perovskite | 2D perovskite | Double perovskite

ACS Energy Lett. 2021, 6, 8, 2750–2754

Properties

- Exceptional electroluminescence (near unity quantum yield)
- High absorption coefficient ($\alpha \sim 10^5$ cm^{-1})
- Tuneable band gaps (~1.7 eV – 2.5 eV)
- Inexpensive fabrication methods

Mixed halide perovskites : Simple mixing in different ratios

RESEARCH ARTICLE

ADVANCED FUNCTIONAL MATERIALS
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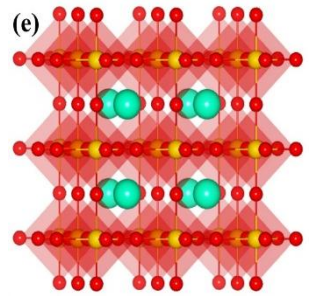
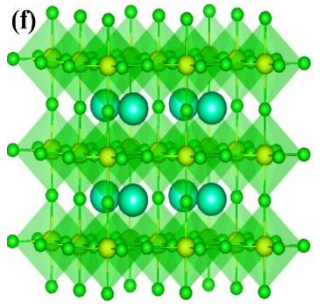
Atomic Insights of Stable, Monodispersed $CsPbI_{3-x}Br_x$ ($x = 0$, 1, 2, 3) Nanocrystals Synthesized by Modified Ligand Cell

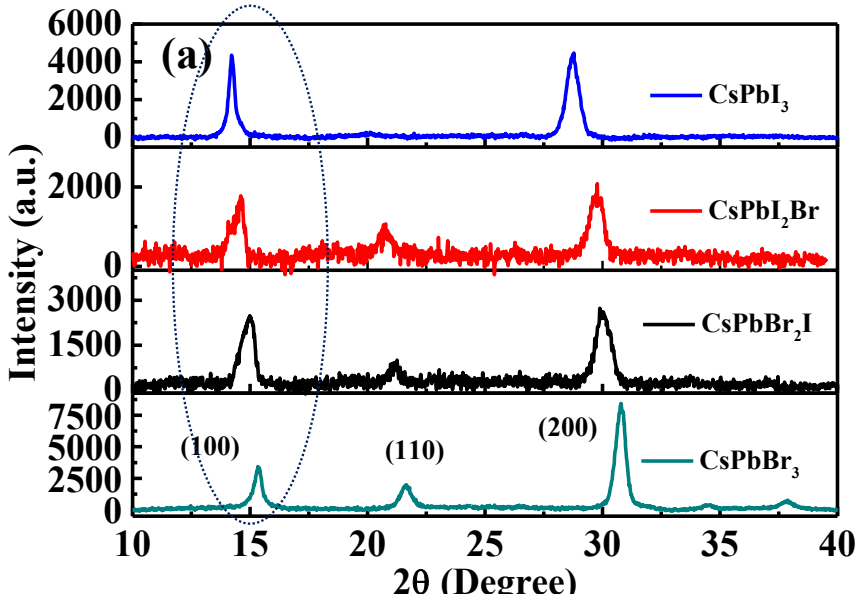
Arup Ghorai, Somnath Mahato, Sanjeev Kumar Srivastava, and Samit K. Ray**

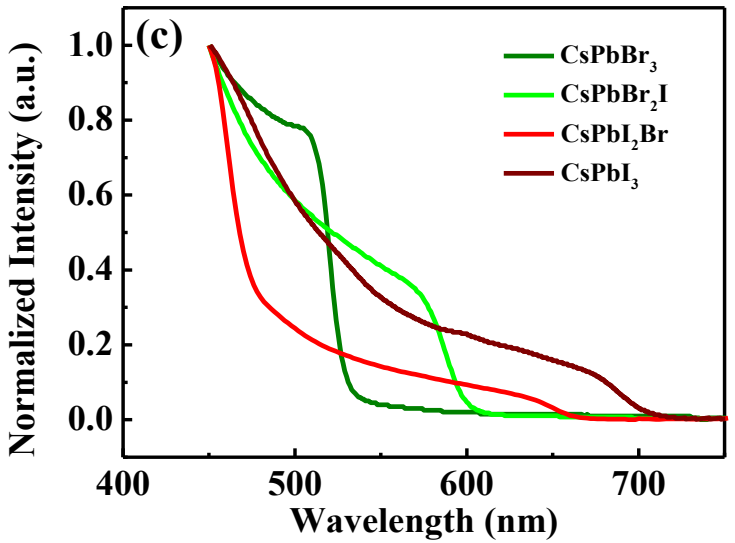


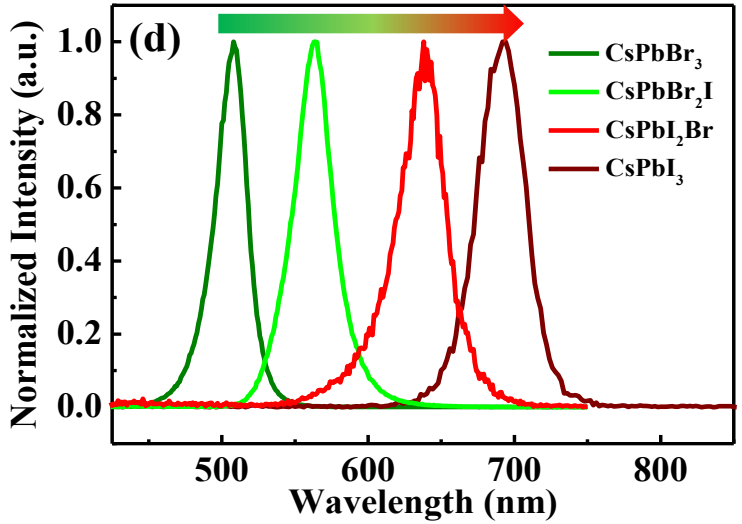
$CsPbI_3$



$CsPbBr_3$







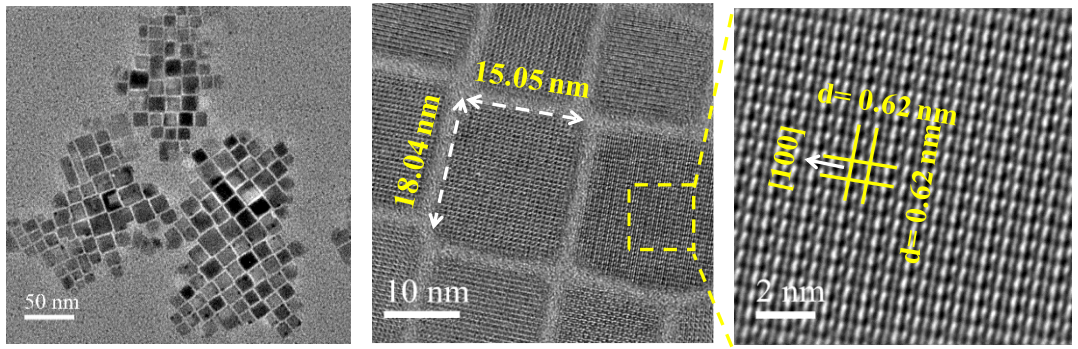
Gradual red shift in absorption and photoluminescence peaks with increase in iodine

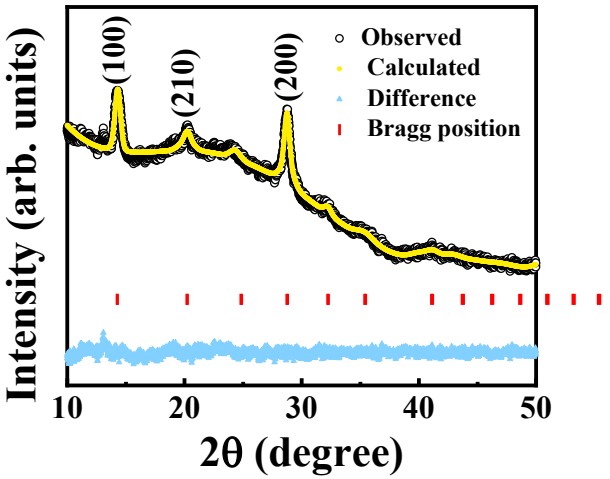
Ghorai et al., Adv. Funct. Mater, 2022, 32, 2202087

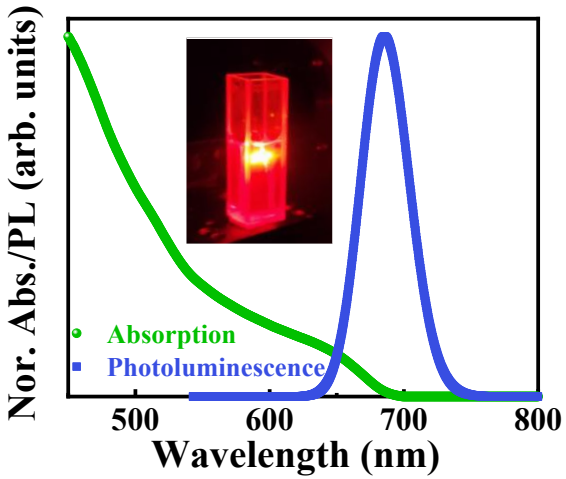
Halide Perovskite Nanocrystals

- Cubic α-$CsPbI_3$: High stability using oleyl amine as a ligand
- Smaller lattice constant : a=6.2315Å

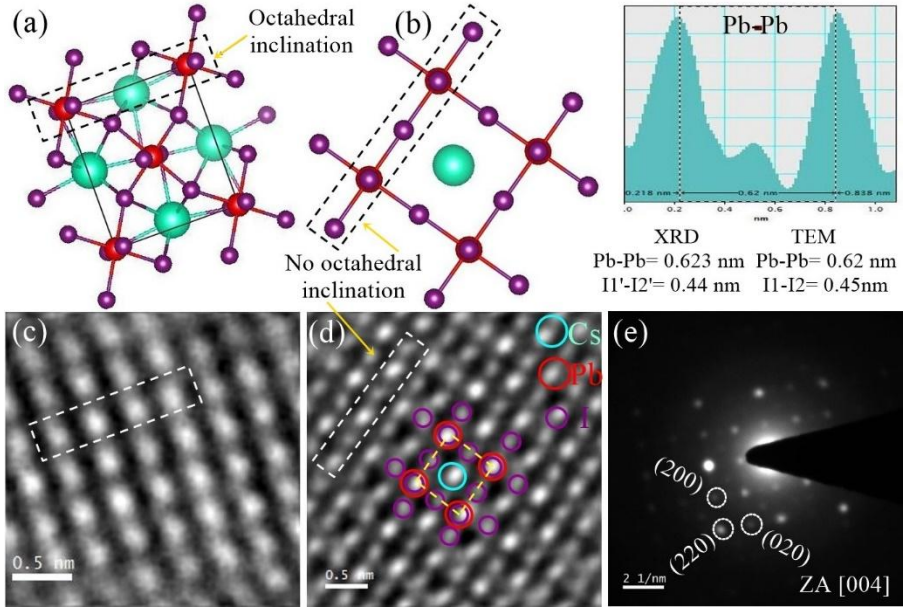
Chemically synthesized of α-phase $CsPbI_3$ NCs







- Structural and optical characteristics of as-synthesised $CsPbI_3$ NCs : Cubic α-phase formation with extended visible photoabsorption up to 700 nm



Atomic positions of Cs, Pb and I

Mahato et al., Advanced Energy Materials, 2001305, (2020)

Ghorai et al., Advanced Functional Mater, 2202087 (2022)

Ghorai et al., Angewandte Chemie, 135, e202302852 (2023)

Bose et al., Appl. Phys. Lett. 124, 011901 (2024)

Mahato et al., Advanced Materials, e03680 (2025)

Talk Outline

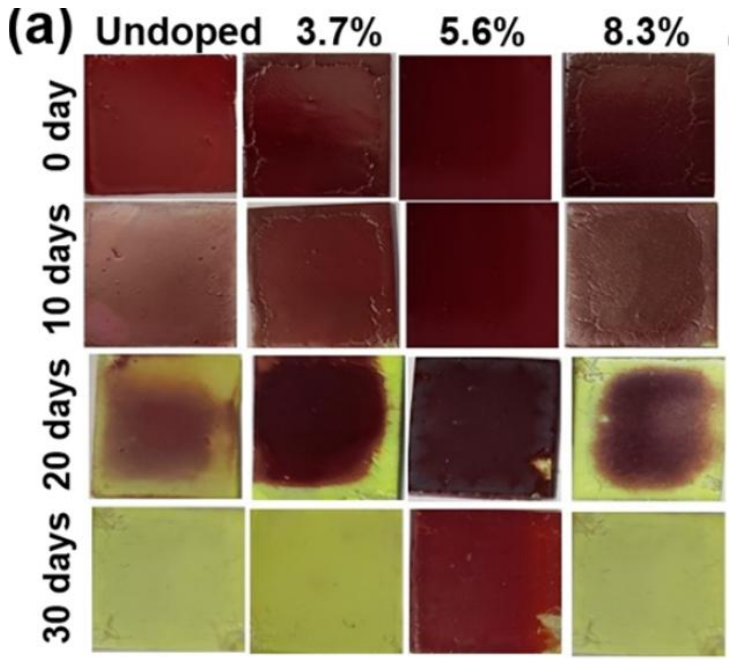
I. $CsPbI_3$ Nanocrystals Sensitized Optoelectronic Devices

- High performance phototransistors
- Nanocrystal sensitized photovoltaic devices

II. Halide Perovskite : Optical & Neuromorphic Devices

- Mixed halide perovskites Light emitting diode (LED) : Effect of R-P faults
- Doping & interface engineered optical synaptic devices

Attempted way to improve device stability



I. B-site Doping

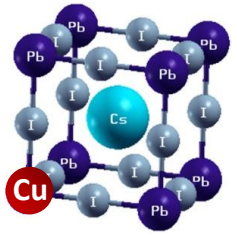
Goldschmidt's tolerance factor

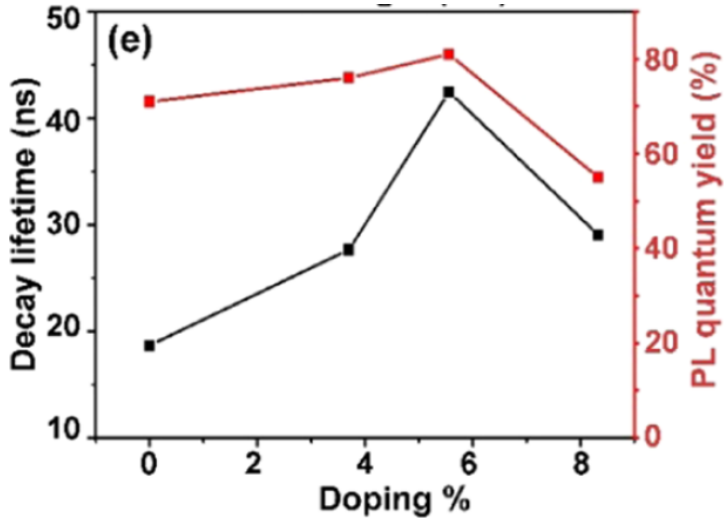
$$\tau = \frac{r_A + r_B}{\sqrt{2}(r_B + r_X)}$$

r_A, r_B, and r_X = effective ionic radii of the A-, B-, and X-site atoms of perovskites (ABX_3)

- Ideally, $\tau \sim 1$
- For $CsPbI_3$, $\tau \sim 0.893$

Cu, t ~ 0.98

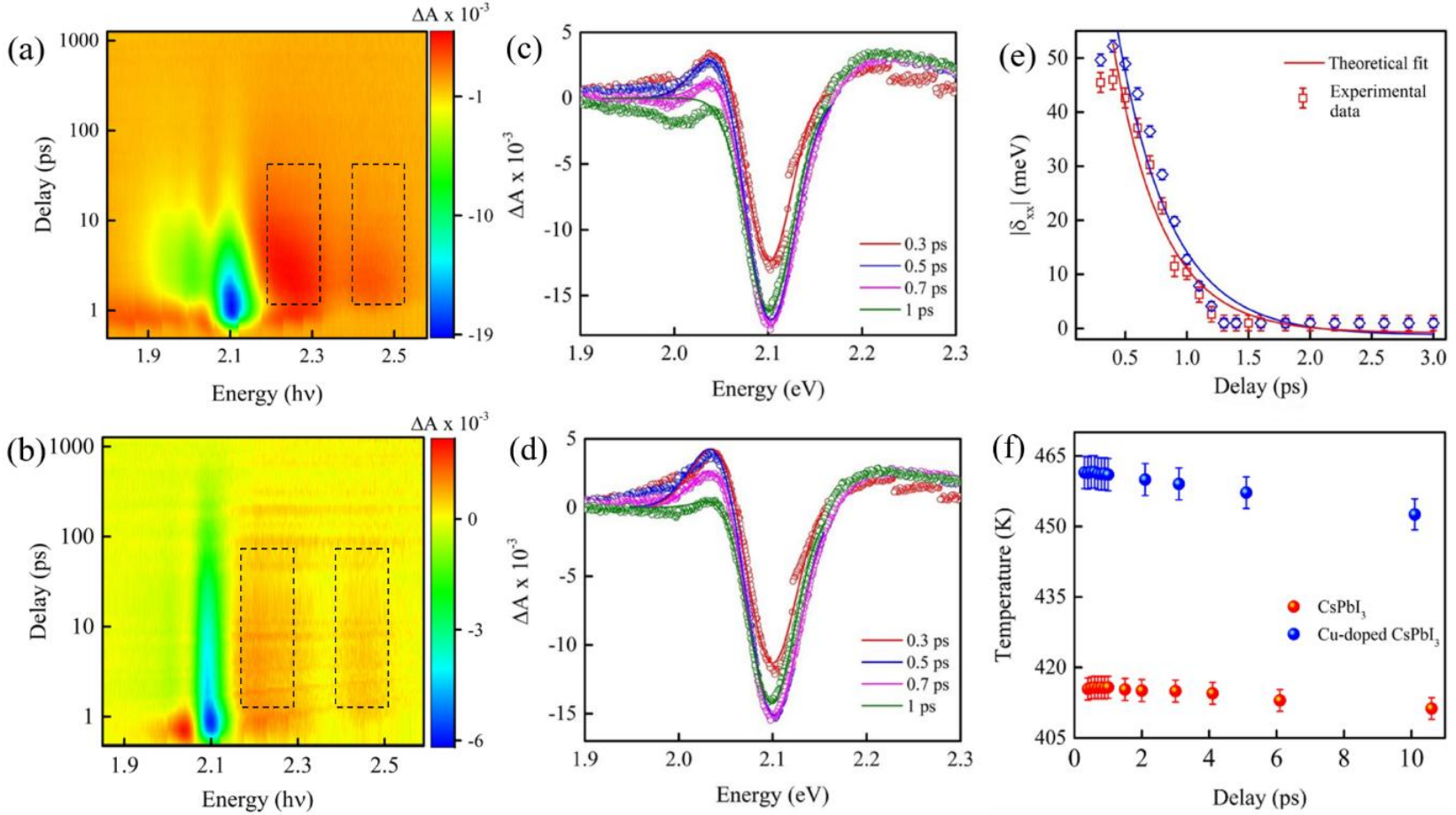




- Doping 5.6% Cu results in maximum enhancement in structural stability of metal halide perovskite $CsPbI_3$
- Film stable for more than 30 days in ambient conditions
- Radiative decay lifetime and photoluminescence yield increases for 5.6% Cu-doping

Roy et al., Chemistry of Materials, 1601 (2023)

Improvement in hot carrier dynamics



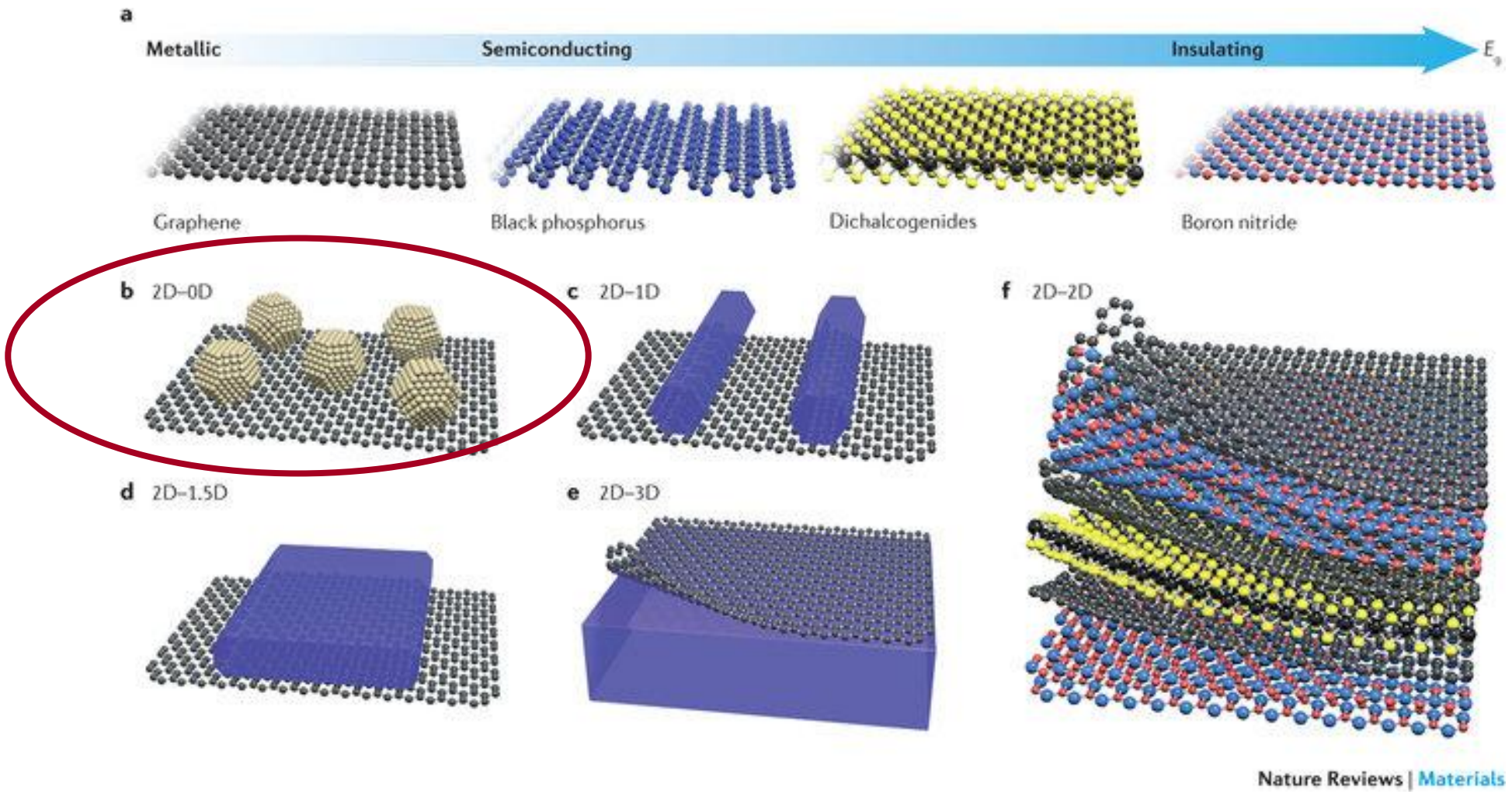
Doping enhances hot carrier energy and thermalization time : suitable for hot-carrier perovskite solar cells

In collaborations with K.V.Adarsh, IISER Bhopal

Bose et al., Appl. Phys. Lett. 124, 011901 (2024)

TA spectrum at a peak intensity of 15 μJ/cm^2 for 3.1 eV pump excitation of (a) undoped and (b) Cu-doped $CsPbI_3$ NCs. Selected cross-section of the contour plots of TA spectrum at $\Delta t \leq 1$ ps for (c) undoped and (d) Cu-doped $CsPbI_3$ NCs. (e) Biexcitonic shift calculated at different delay times for undoped and Cu-doped $CsPbI_3$ NCs. (f) Carrier temperature: At time, Δt <1 ps, carriers at ~461 K and ~415 K for doped system and $CsPbI_3$, respectively.

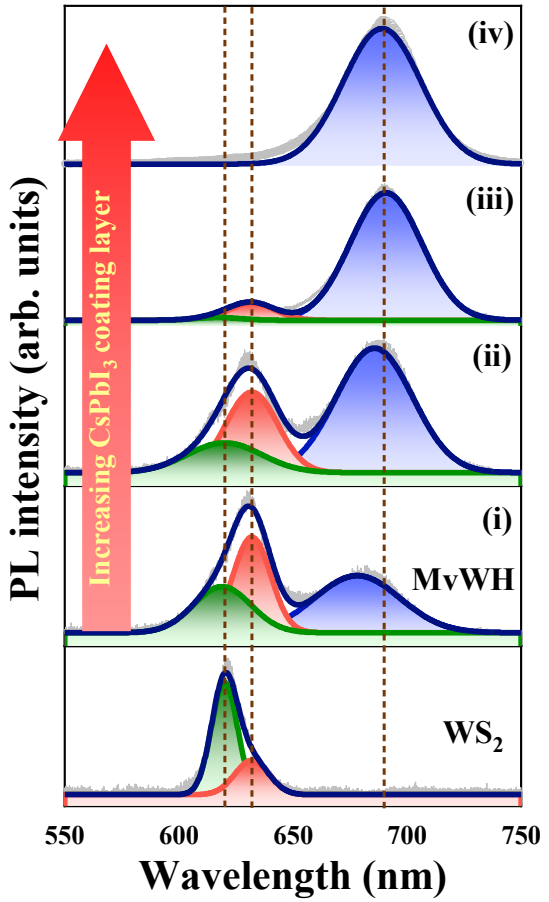
Mixed-dimensional Heterostructures

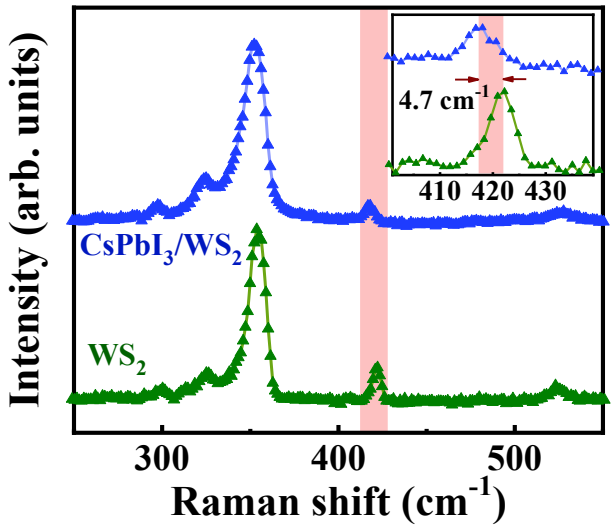


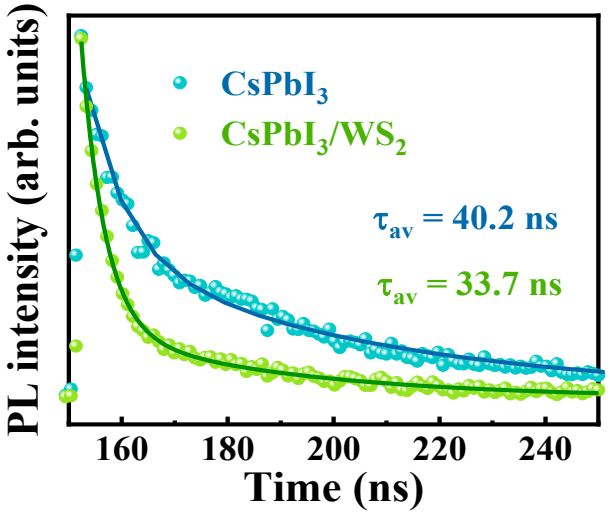
Achieve 2D/nD Heterostructures for Si-CMOS Compatible Photonic Applications

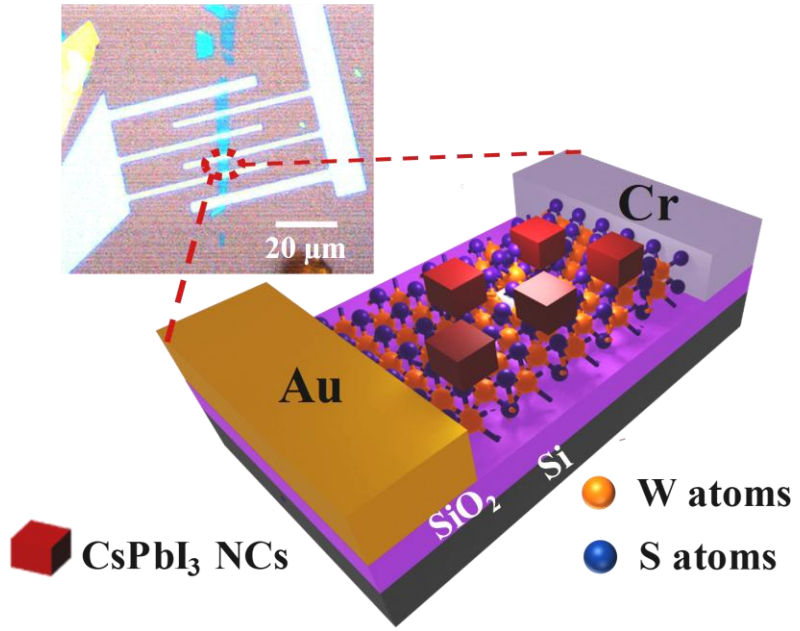
I. $CsPbI_3$ NCs/WS_2 (0D/2D) Heterojunction Phototransistor

Charge transfer mechanism in heterostructure samples





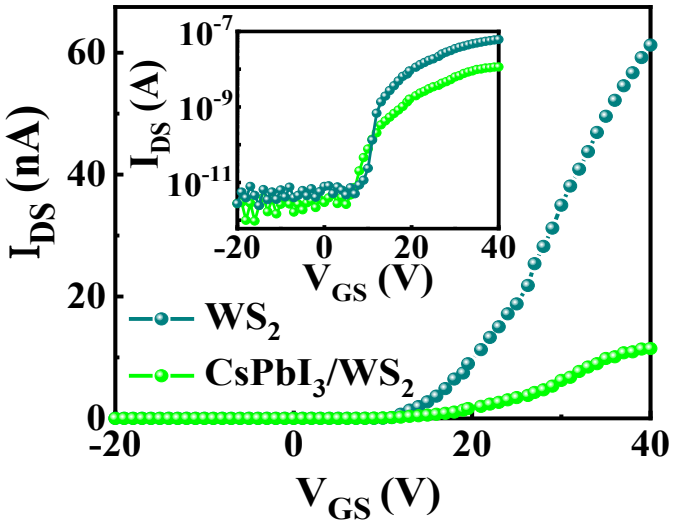


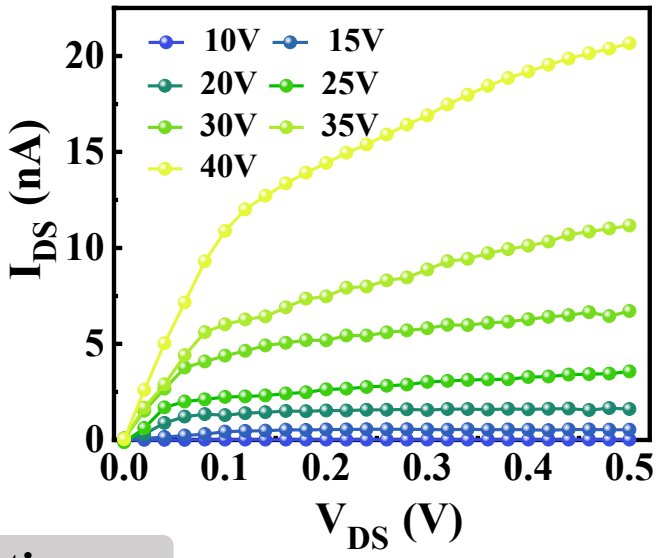


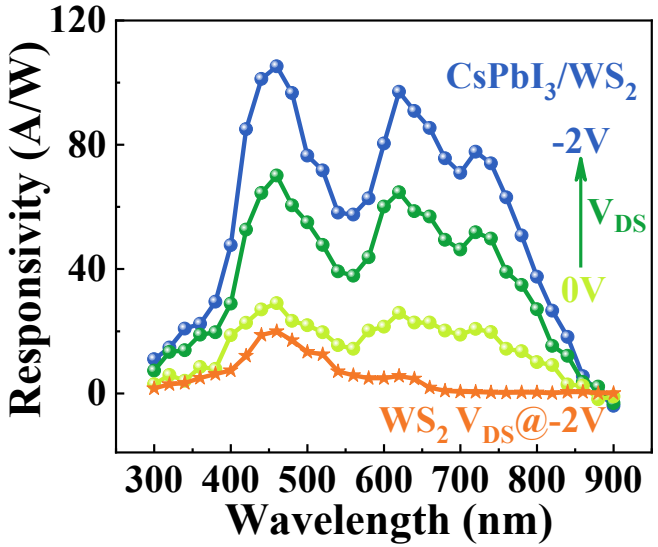
- WS_2 excitonic peak quenches
- WS_2 trionic peak enhancement
- Overall $CsPbI_3$ PL peak quenches

Das et al., Physical Review Applied 19.3 (2023): 034051.

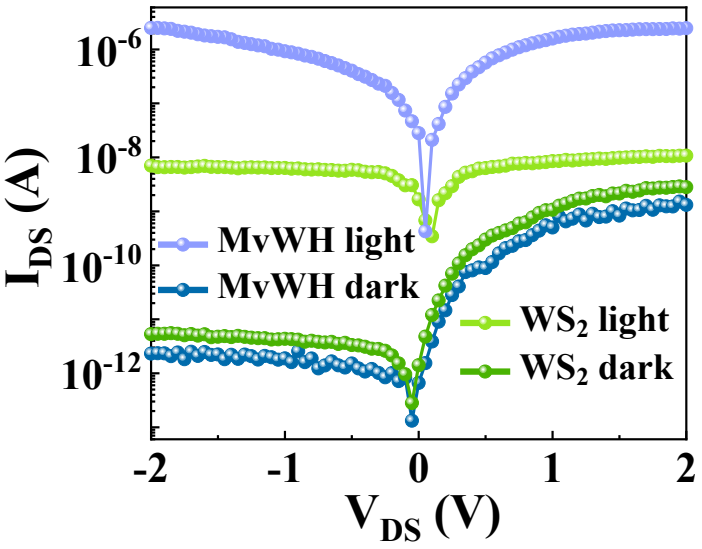
QDs Sensitized WS_2 Phototransistor with asymmetric contacts







Photoresponse characteristics



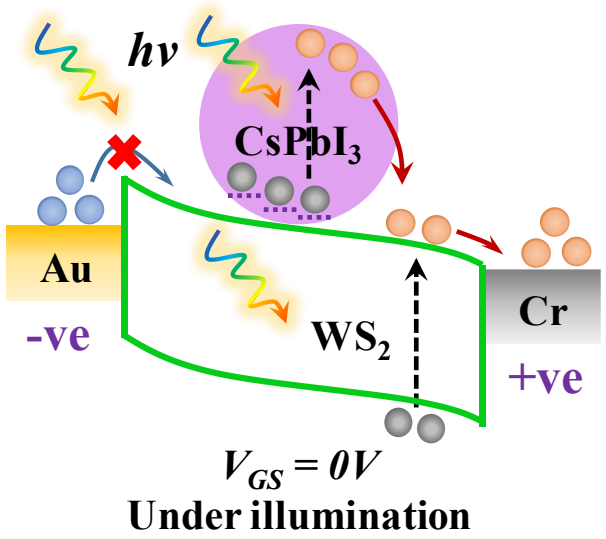


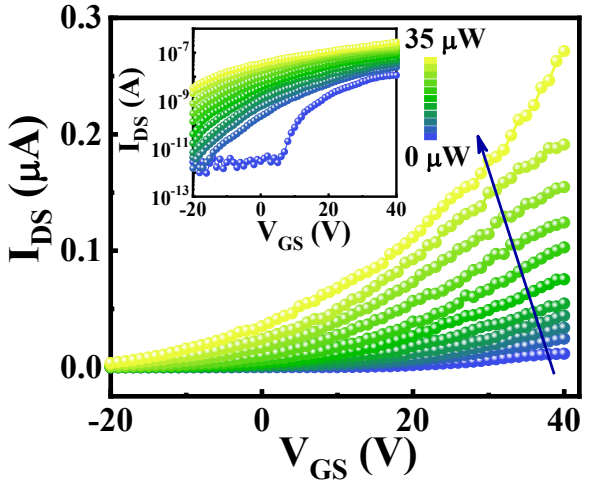
Photo-FET at zero gate bias: Enhanced & extended spectral response up to 900 nm

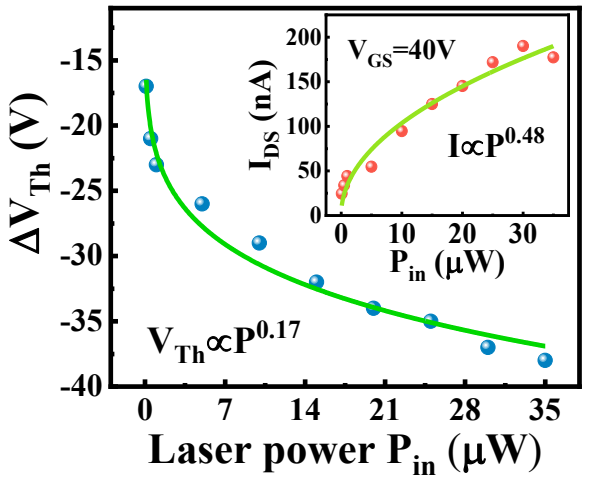
Photo-to-dark current ratio: ~10^6 for $CsPbI_3/WS_2$

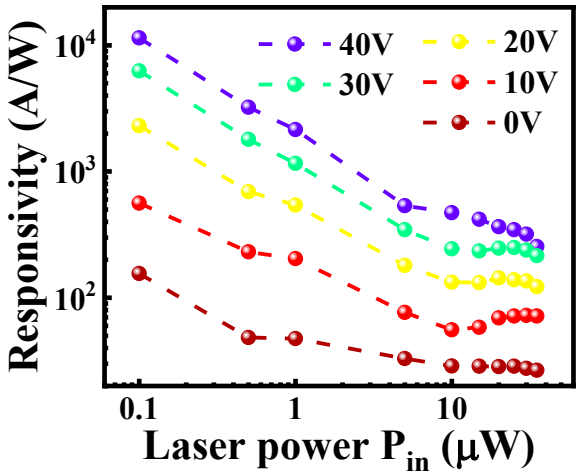
Das et al., Physical Review Applied 19.3 (2023): 034051.

Gate tunable phototransistor characteristics

Strong photo gating effect from trapped holes inside $CsPbI_3$ NC sensitizers

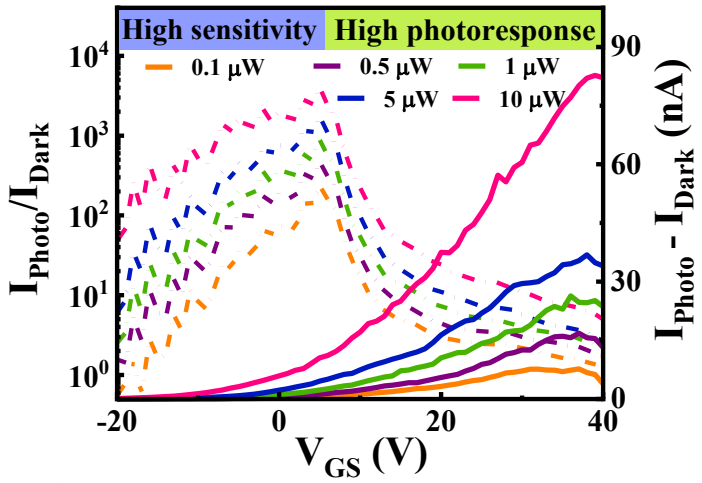


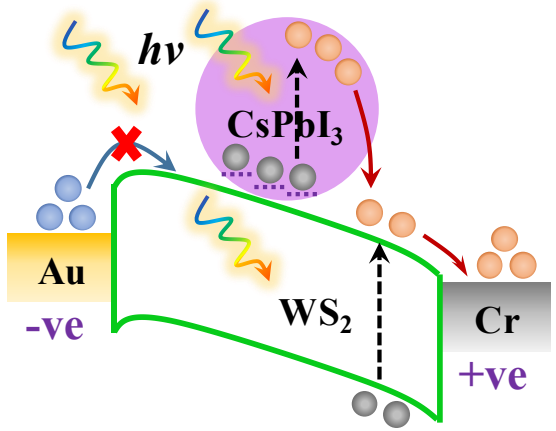




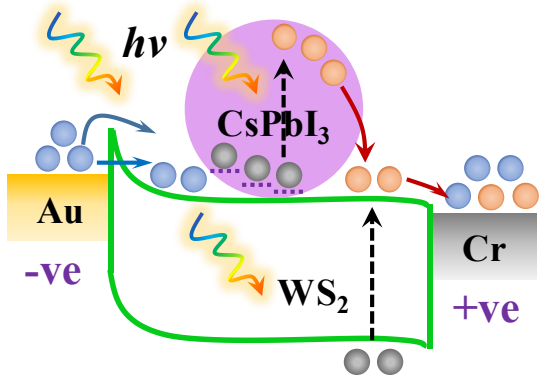
- The maximum responsivity ~ 10^4 A/W at V_{GS}=40V
- The detectivity is ~ 1.2 × 10^{13} Jones.

Gate tunable photo-FET performance: from high sensitivity to high photoresponse





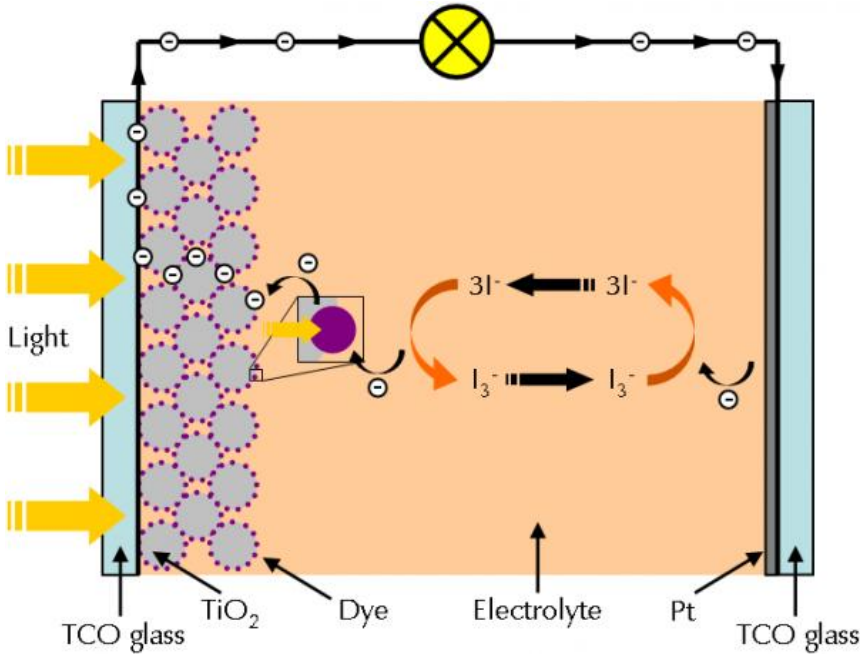
$V_{GS} < V_{Th}$
Depletion region

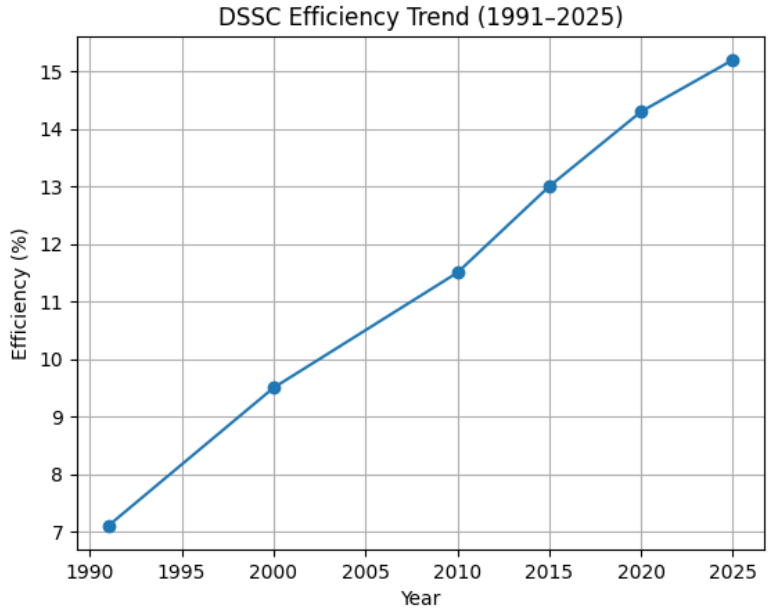


$V_{GS} > V_{Th}$
Accumulation region

Das et al., Physical Review Applied 19.3 (2023): 034051.

II. Perovskite NCs Sensitized PV Devices





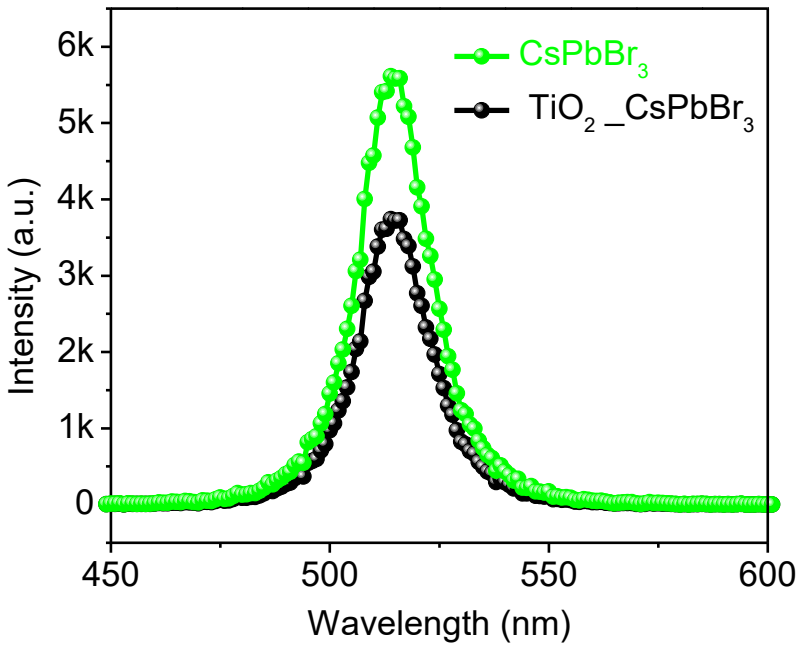
Limitations of DSSCs :

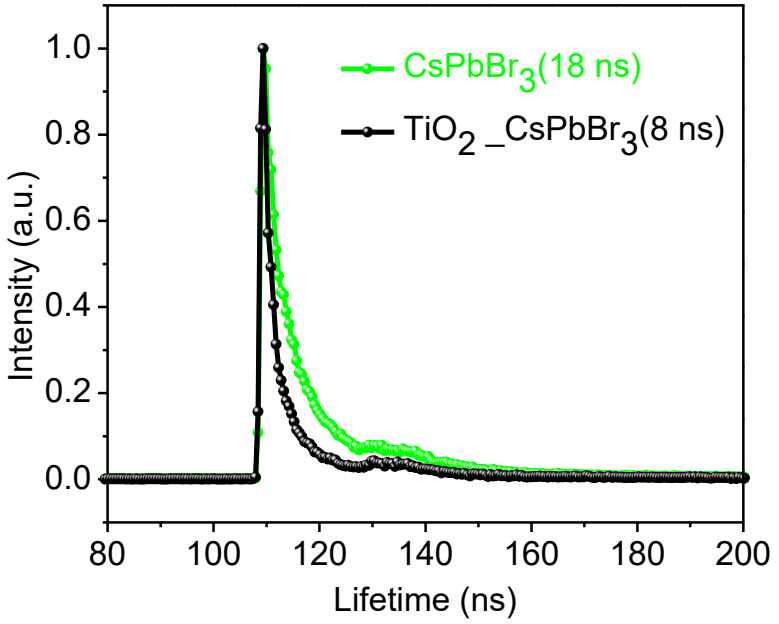
- Dyes degrade under UV and prolonged light exposure
- Dye molecules can aggregate on TiO_2 surface
- Slow electron injection
- Structural changes reduce performance

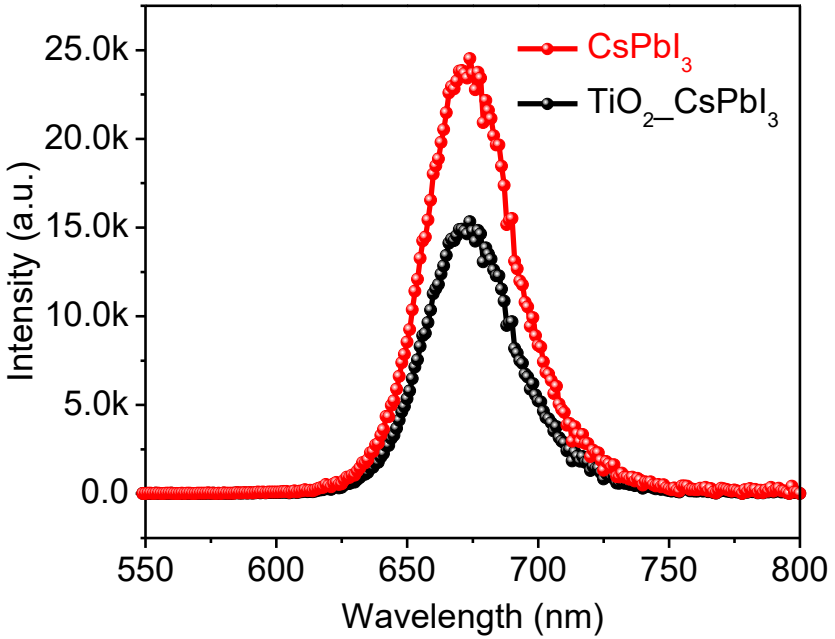
Nanocrystal Sensitizers :

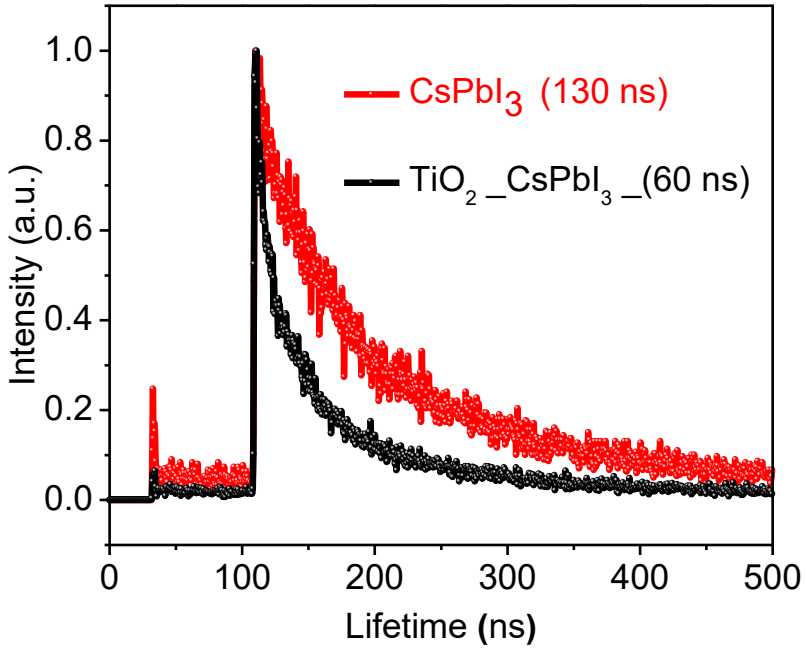
- Higher absorption coefficient (~10^5 cm^{-1})
- High carrier mobility and long diffusion lengths (~1 µm)
- Tunable bandgap (1.2–2.3 eV) by changing halides (I, Br, Cl)

Perovskite NCs Sensitizers

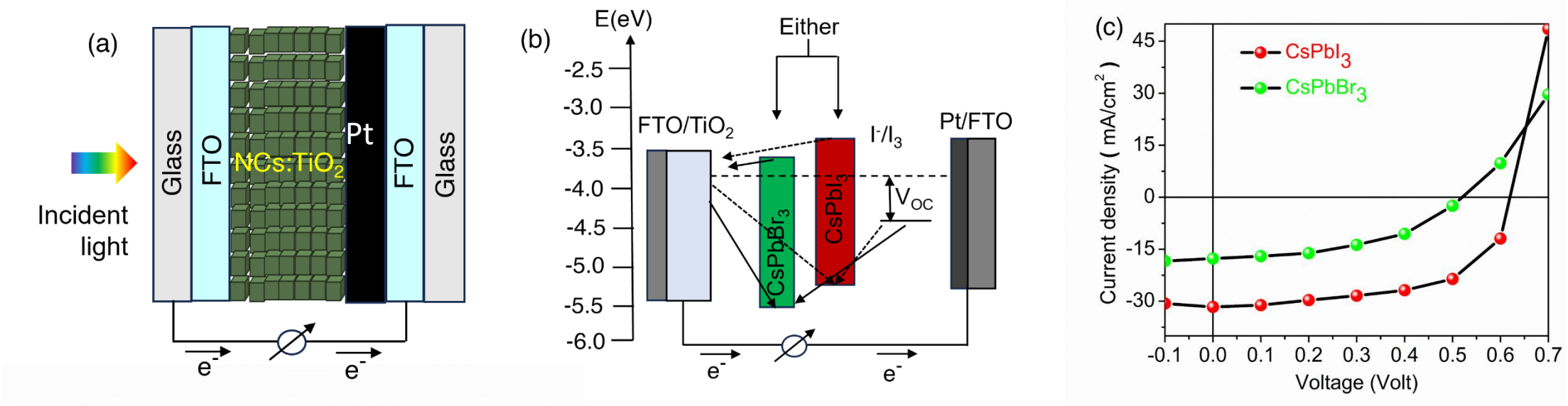


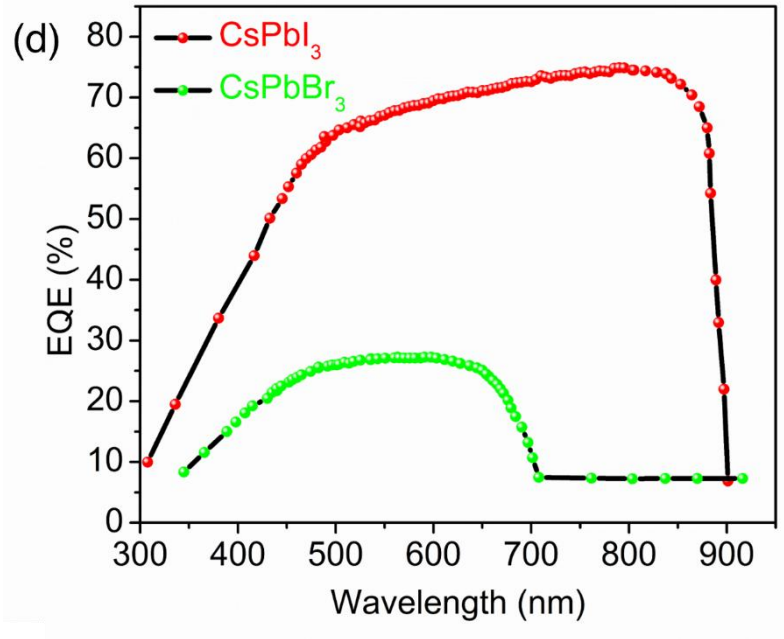






Perovskites NCs-sensitized solar cells

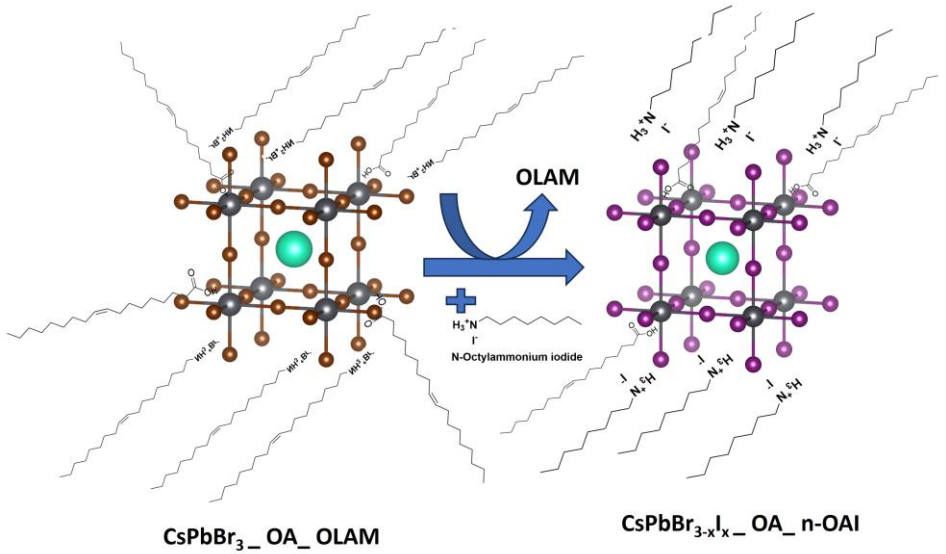


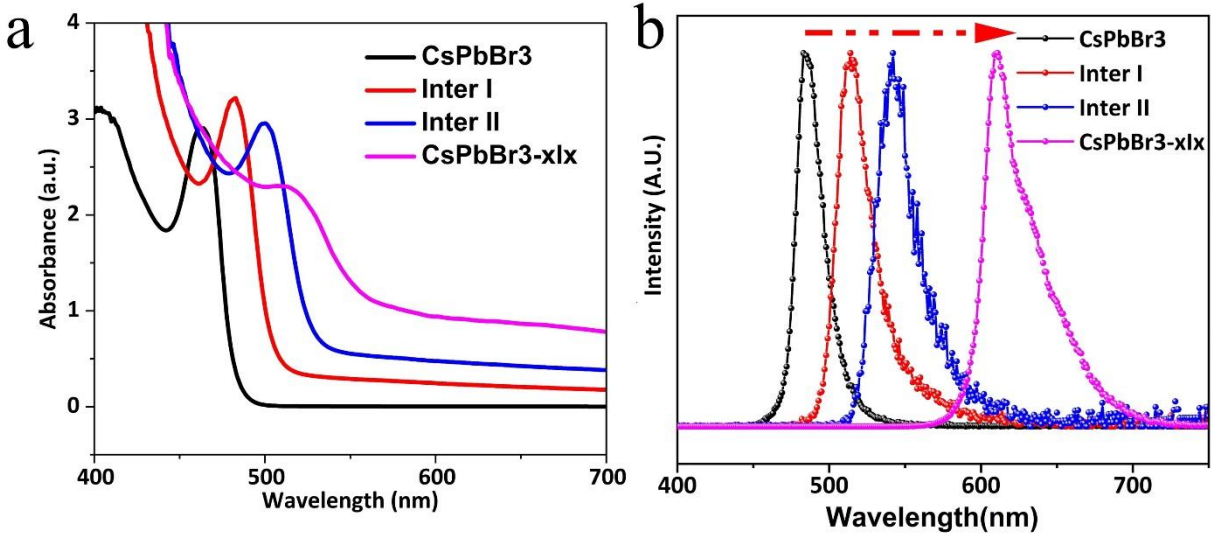


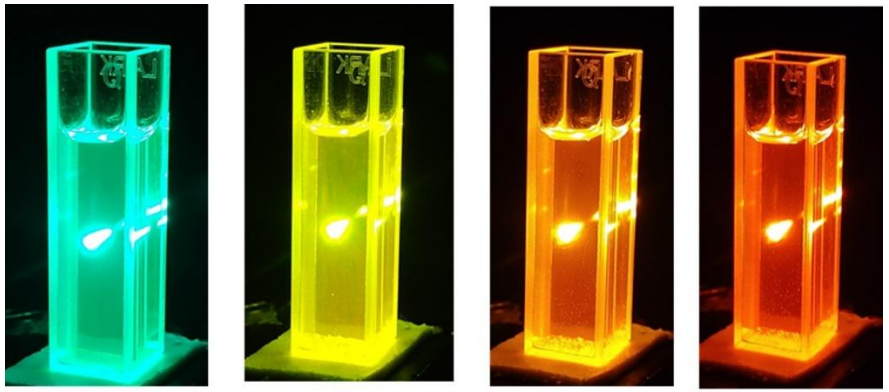
Active materials	J_{sc} (mA/cm²)	V_{oc} (V)	FF (%)	PCE (%)
$CsPbBr_3$	18.1	0.52	42	3.9 %
$CsPbI_3$	32.1	0.61	64	12.5 %

Roy et al., Nanoscale, 10743 (2025)

III. Anion Exchanged Mixed Halides : LEDs

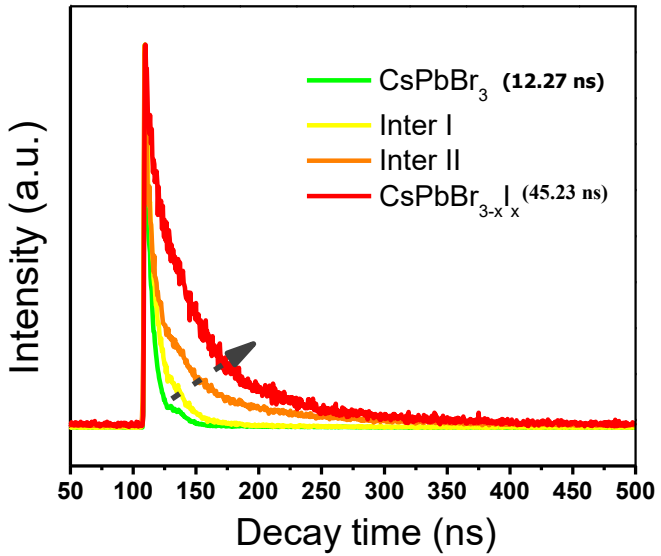






$CsPbBr_{3-x}I_x$

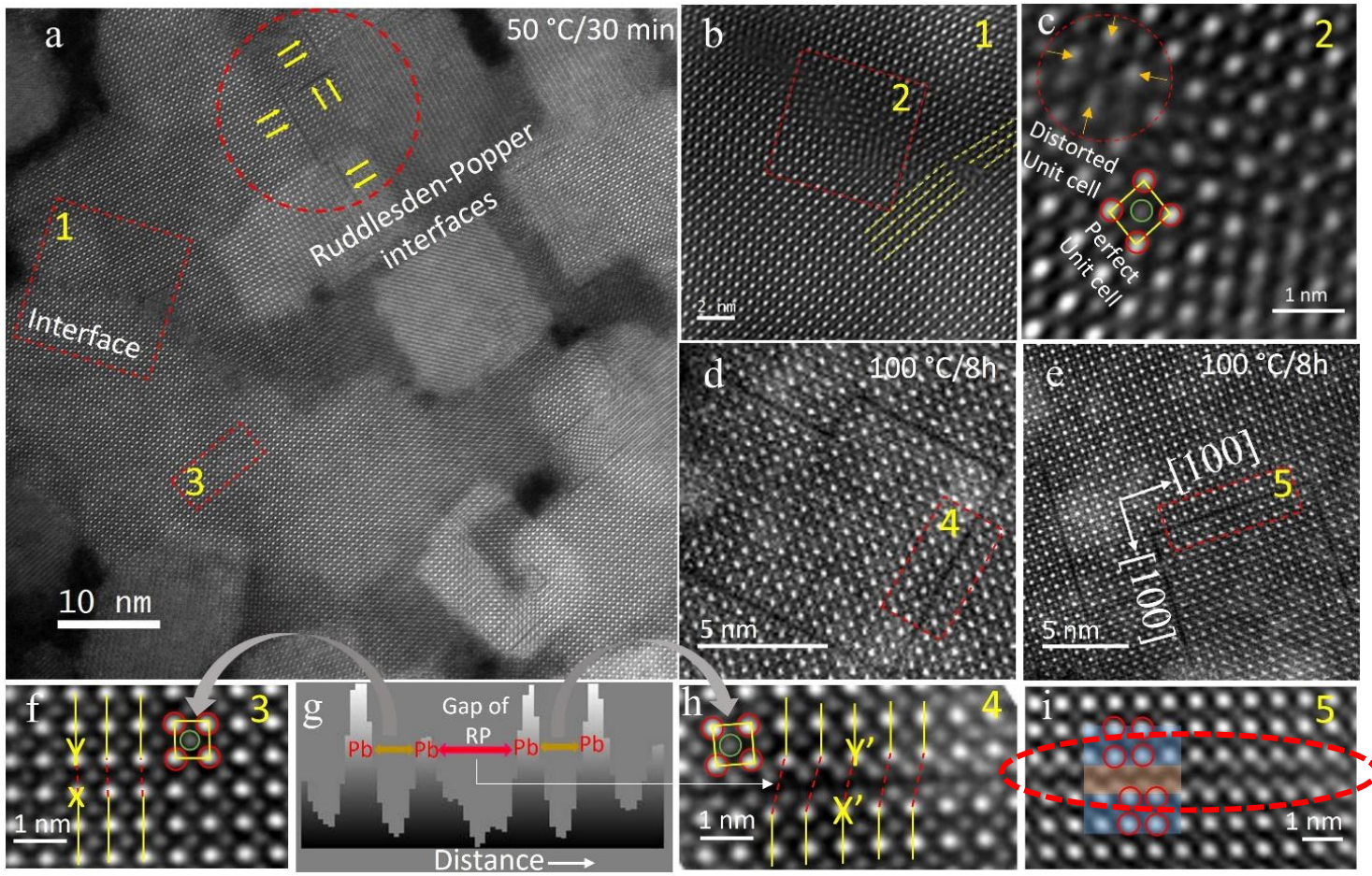
n-octylammonium Iodide



Video of $CsPbBr_3$ to $CsPbBr_{3-x}I_x$

MHPs : 2D Ruddlesden - Popper (RP) Faults

HAADF-STEM images of ligand-treated $CsPbBr_3$



- ✓ RP faults accommodate misfit and strain
- ✓ Prevents ion migration
- ✓ Can localize carriers – carrier confinement
- ✓ Increased probability of recombination

atomic misfits

Mahato et al. Advanced materials, e03680, 2025

From flaws to functional assets : RP faults for light emission

Perovskite-info

3PATAT-C3 TCI
Efficient Charge Recovery from Perovskite Layer

Researchers turn flaws in perovskite crystals into functional assets

In the world of materials science, defects are u: seen as problems, unwanted microscopic fea that degrade performance, redu[ce] effici[ency], the life span of devi[ces]. [A] recent stuc scientists from Łuka[sie]wicz Research Network – Polish Centre for Technology Development Indian Institute [of] Technology Kharagpur challenged this perception.

MEDIA NEWS

nanowerk.com

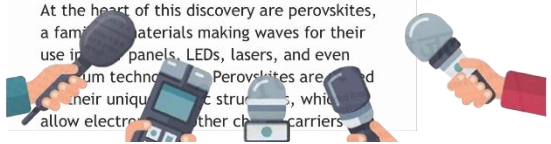
Aug 08, 202[5]

When flaws become feature[s]: Turning defects into brighter perovskite emission

Engineered atom[ic] faults in perovskites boost light [output] nearly 80 percent and improve stability, offering new design strategies for brighter, more durable optoelectronic devices.

(*Nanowerk News*) In the world of materials science, "defects" are usually the bad guys, tiny imperfections in a material's structure that sabotage performance, drain efficiency, or shorten a device's life span. But a new study published in *Advanced Materials* ("Atomically Precise Ruddlesden-Popper Faults Induced Enhanced Emission in Ligand Stabilized Mixed Halide Perovskites") flips this idea on its head. It reveals how a long-misunderstood defect in crystals, known as the Ruddlesden-Popper (RP) fault, could be the secret ingredient to unlocking brighter and more stable light-emitting materials.

At the heart of this discovery are perovskites, a fami[ly] [of] materials making waves for their use in [solar] panels, LEDs, lasers, and even [quantum] techno[logy]. Perovskites are [valued] for their uniqu[e] [crystal] stru[cture], whi[ch] allow electr[ons] [and] other ch[arge] carriers



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AUGUST 11, 2025 DIALOG — The GIST

Rethinking imperfections: How defects are powering brighter perovskite emissions

by Somnath Mahato and Muhammad Danang Birowosuto

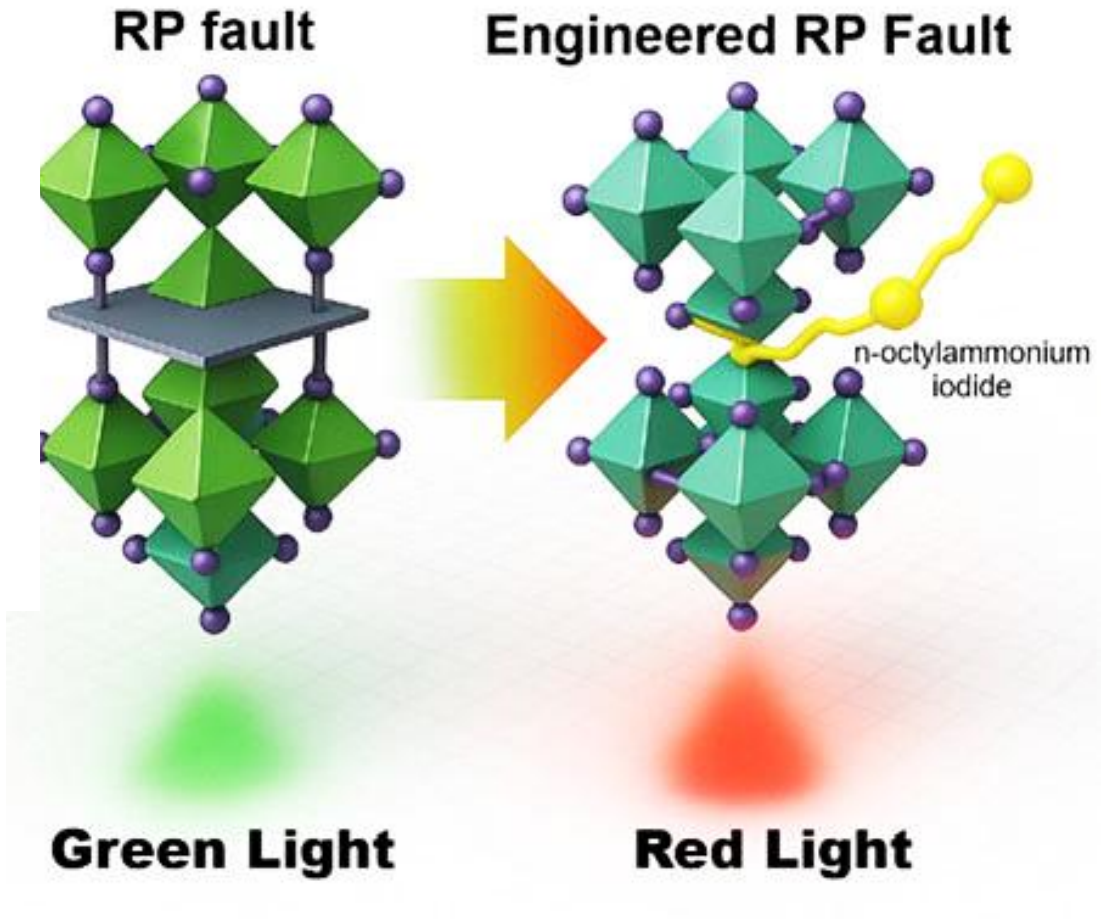
edited by Lisa Lock, reviewed by Robert Egan — Editors' notes

RESEARCH ARTICLE

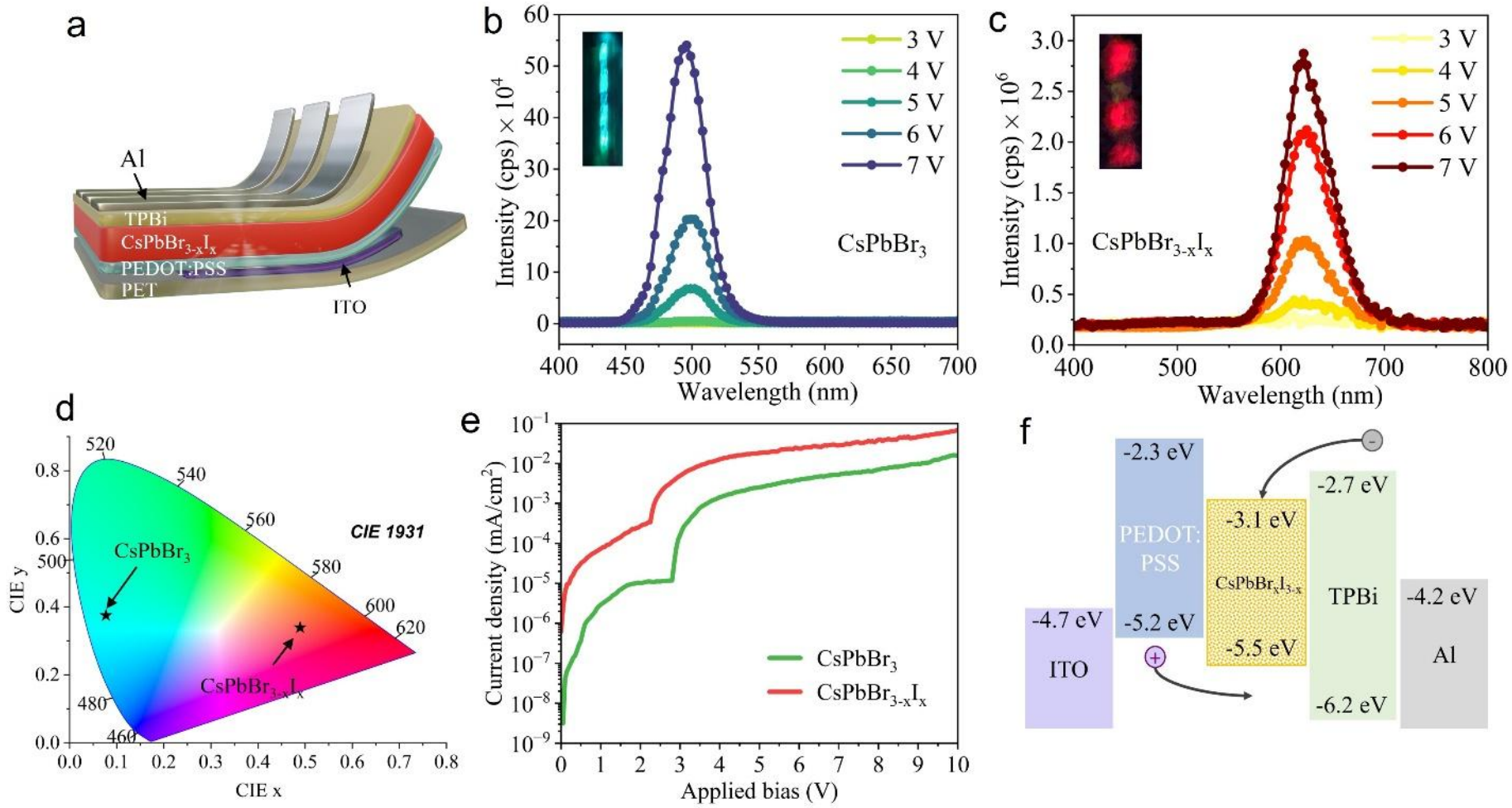
ADVANCED MATERIALS
www.advmat.de

Atomically Precise Ruddlesden–Popper Faults Induced Enhanced Emission in Ligand Stabilized Mixed Halide Perovskites

Somnath Mahato, Baidyanath Roy, Shaona Bose, Satayender K. Sangwan, Narayan Chandra Das, Muhammad Danang Birowosuto, and Samit K. Ray**



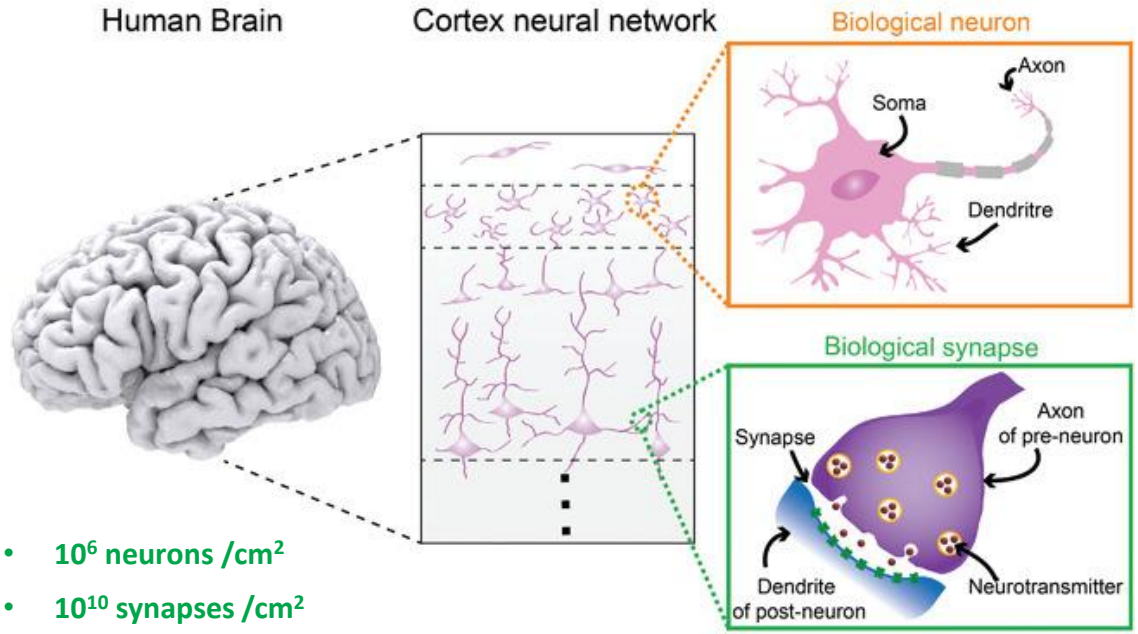
LEDs : Using NOAI-induced RPFs

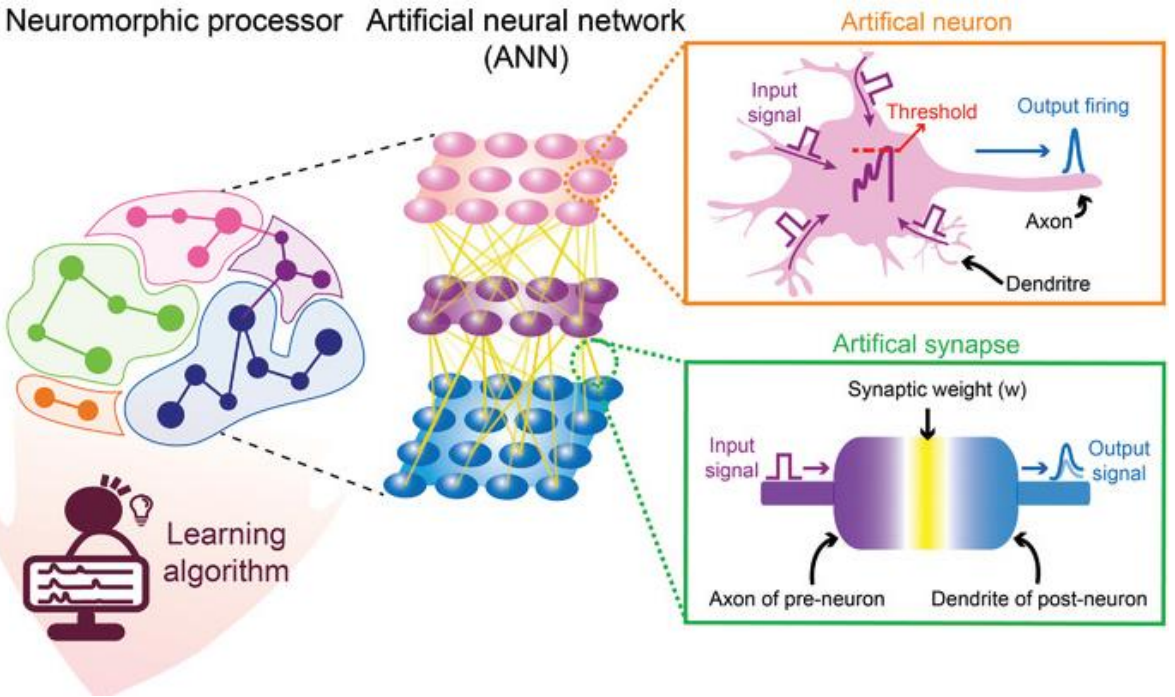


Electroluminescence intensity increased by 80%!

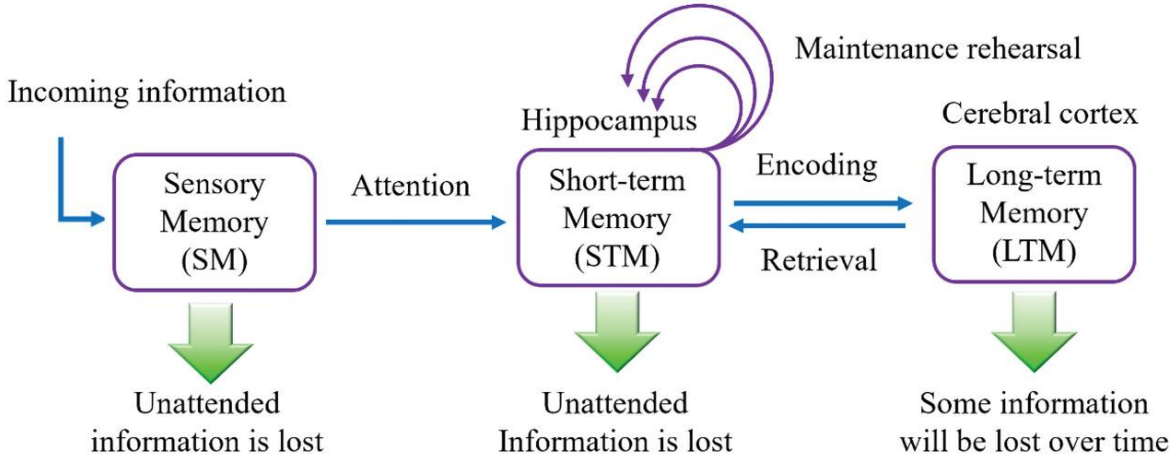
Mahato et al. Advanced materials, e03680, 2025

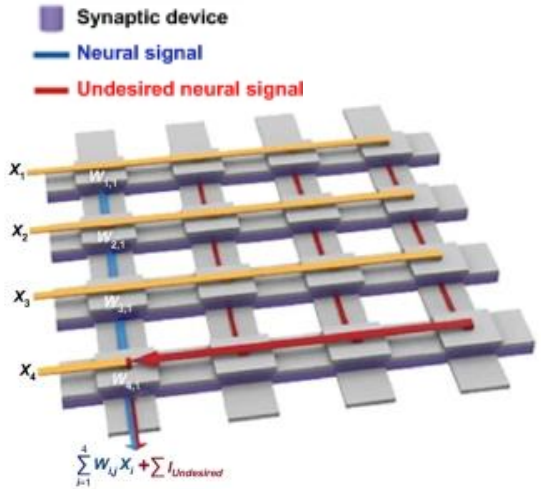
IV. Brain-inspired (Neuromorphic) Devices

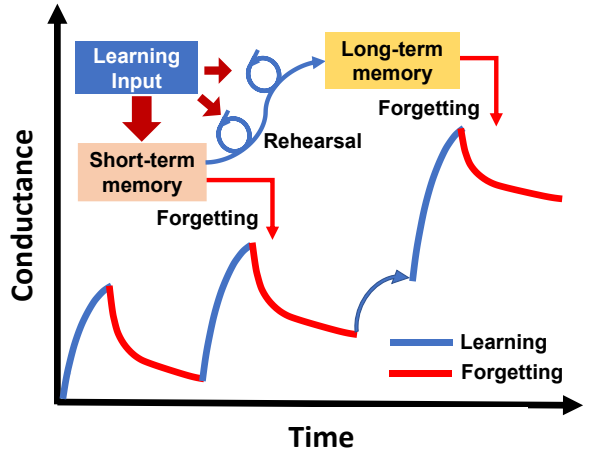




- 10^6 neurons /cm^2
- 10^{10} synapses /cm^2
- Total power consumption: 20 Watts



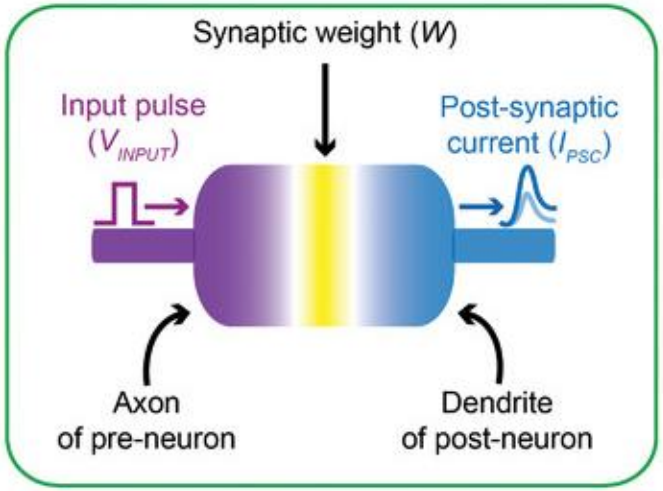




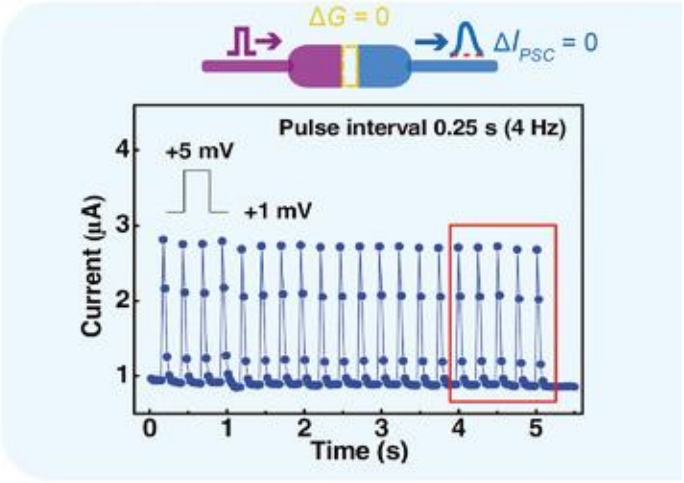
Adv. Mater.2020, 32, 2004659
Nano-Micro Lett. (2022) 14:58

Essential Functions of Artificial Synapses

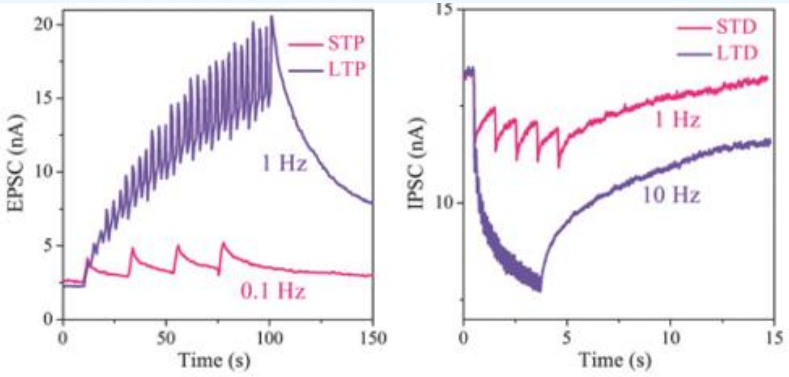
Representative synaptic functions



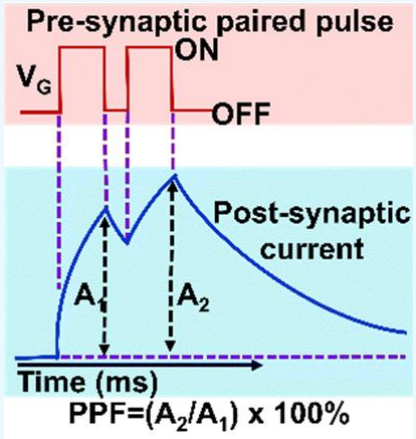
Short-term plasticity (STP)



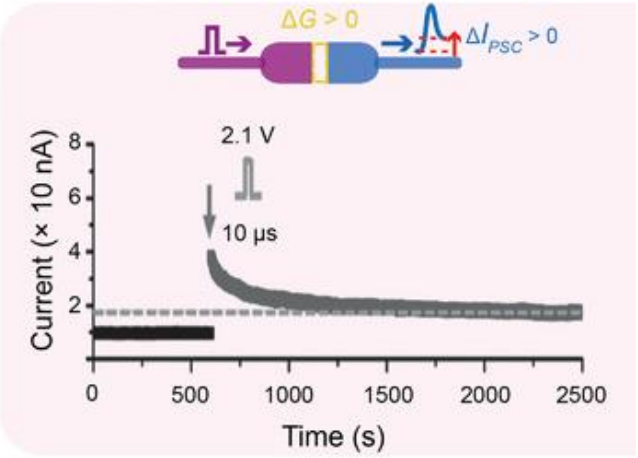
Spike rate-dependent plasticity (SRDP)



Paired pulse facilitation (PPF)



Long-term potentiation (LTP)



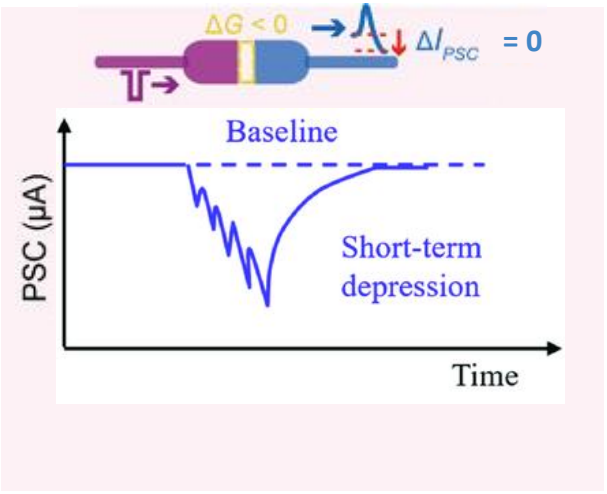
- **Synaptic weight regulation:** Increase in synaptic weight (potentiation) and decrease in synaptic weight (depression)
- **Short-term plasticity:** Temporal increase of synaptic weight
- **Long-term potentiation:** Permanent change in synaptic weight
- **Spike rate-dependent plasticity:** Synaptic weight variance as a function of spiking rate
- **Paired pulse facilitation (PPF):** Current changes between the adjacent pulses.

Adv. Mater.2020, 32, 2004659

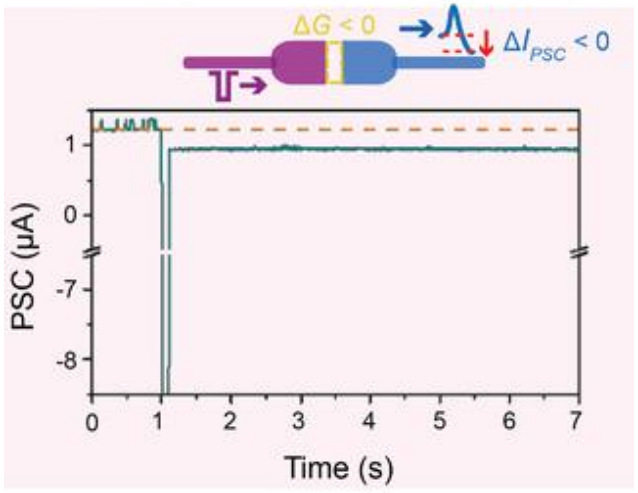
J. Mater. Chem. C, 2024, **12**, 5299-5338

Essential Functions of Artificial Synapses

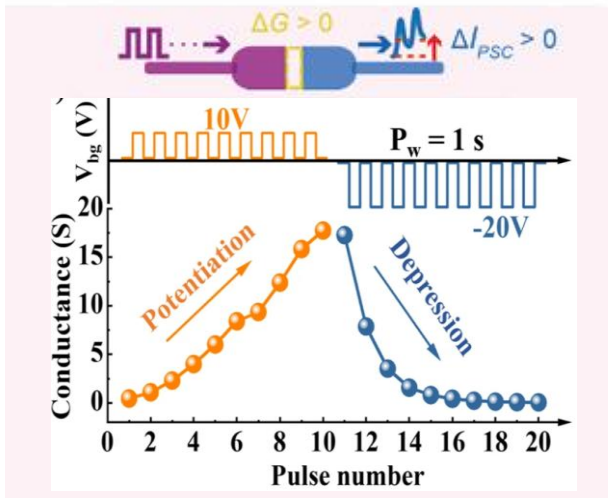
Short-term depression (STD)



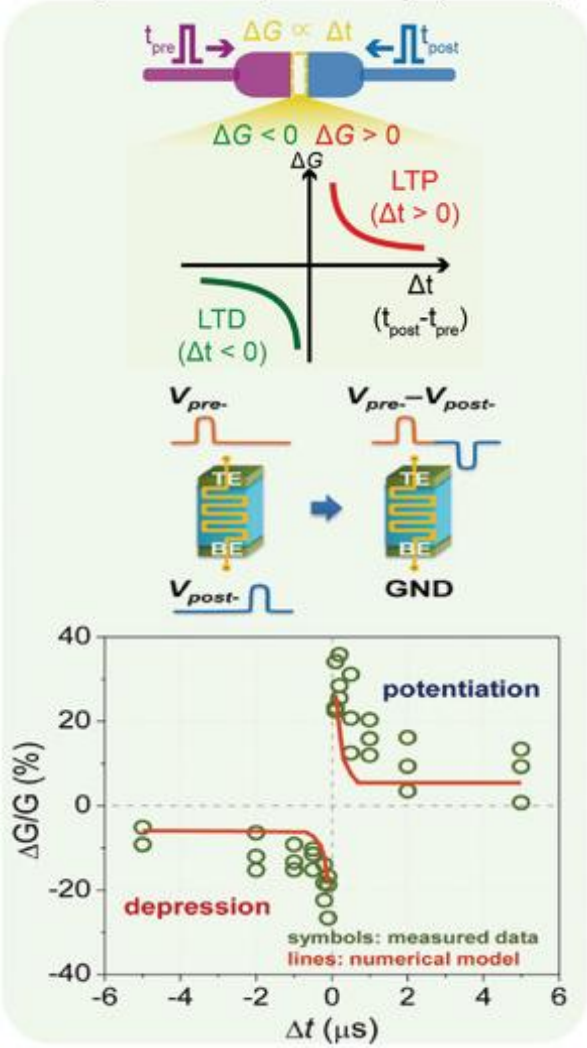
Long-term depression (LTD)



Consecutive LTP & LTD



Spike-timing -dependent-plasticity (STDP)

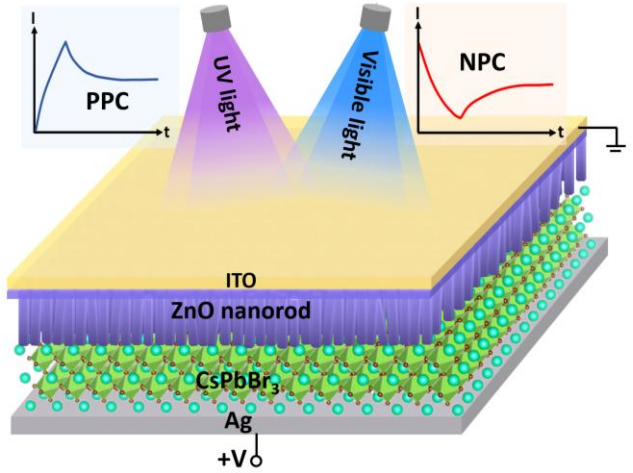


- **Short-term depression (STD):** Temporal decrease of synaptic weight
- **Long-term depression (LTD):** Permanent low value of synaptic weight
- **Consecutive LTP and LTD:** This emulation can be controlled by a pulse train consisting of potentiating and depressing pulses, causing an analog change in the synaptic weight.
- **Spike timing-dependent plasticity (STDP):** Synaptic weight variance as a function of spiking time difference between the firing of the pre- and post-synaptic neurons.

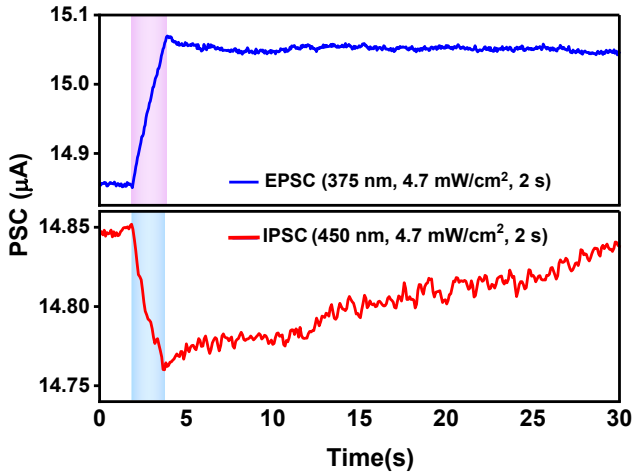
Adv. Mater.2020, 32, 2004659

npj 2D Mater Appl **7**, 63 (2023)

Bidirectional Photoresponse in Perovskite/Oxide Heterojunction

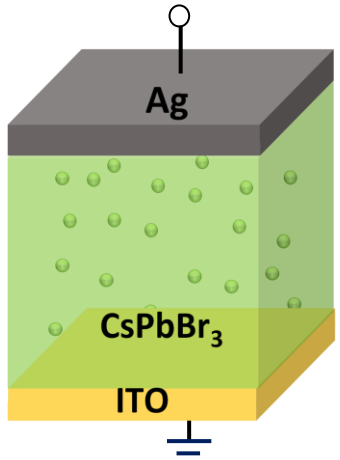


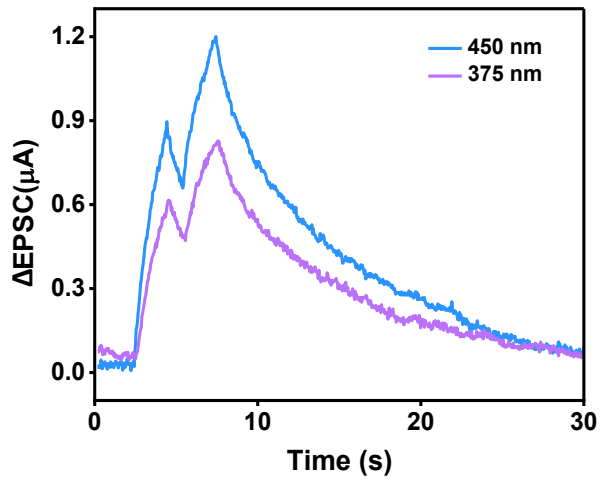
Excitatory & Inhibitory-synaptic behaviour

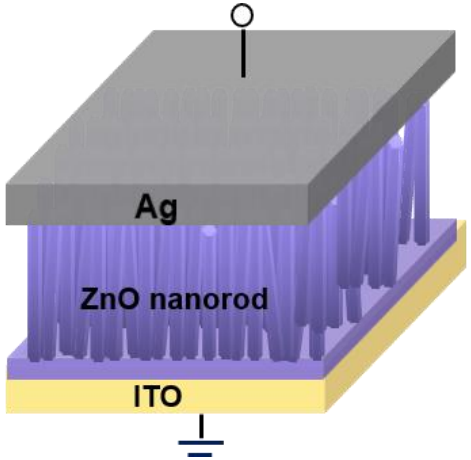


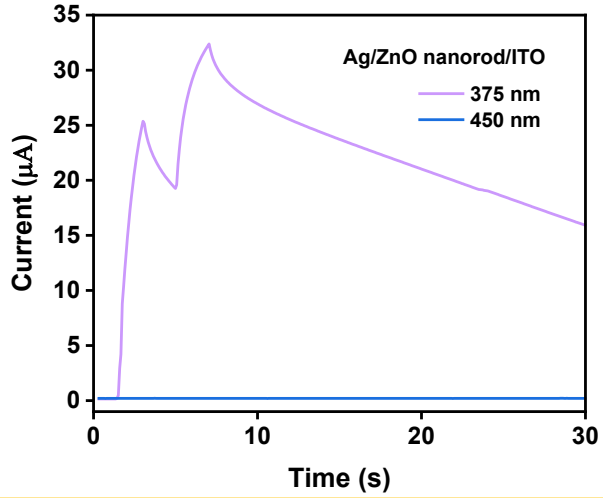
❖ **Positive photo-conductance (PPC) for 375 nm and negative photo-conductance (NPC) for 450 nm light pulses.**

Control Devices





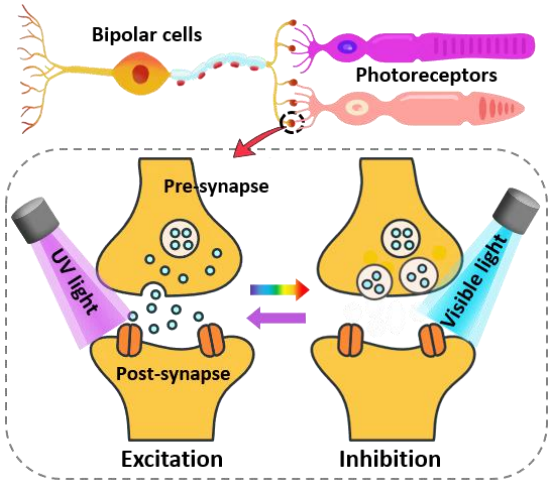




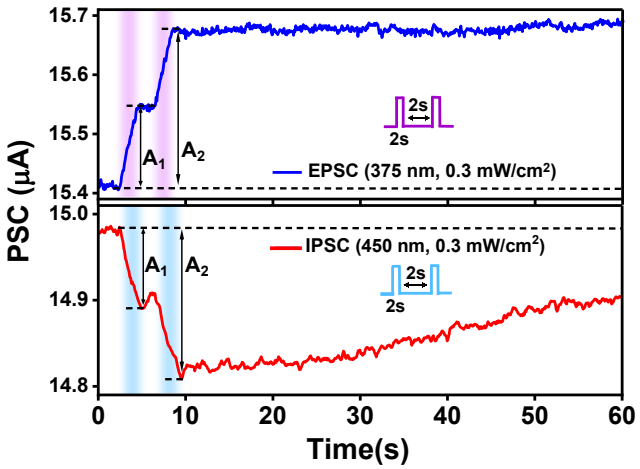
❖ **$CsPbBr_3$-only devices show PPC nature in all wavelengths.**

❖ **ZnO-only devices show PPC nature in 375 nm but show negligible response in 450 nm wavelength.**

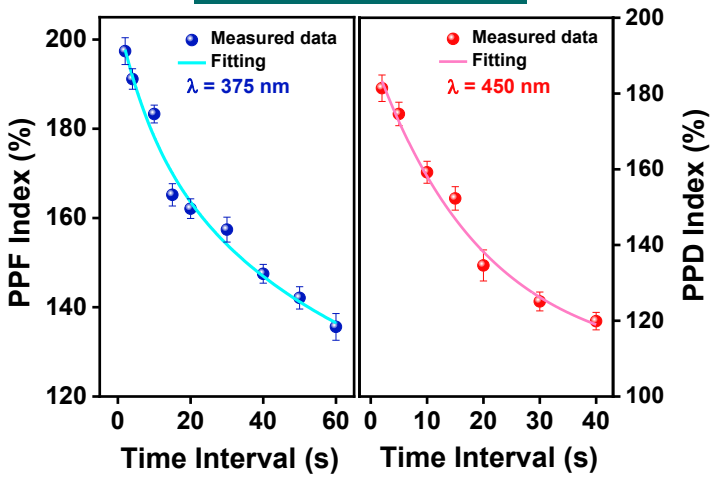
Mimicking fully light-controlled Excitatory & Inhibitory Synapses



PPF & PPD behavior



PPF & PPD Index

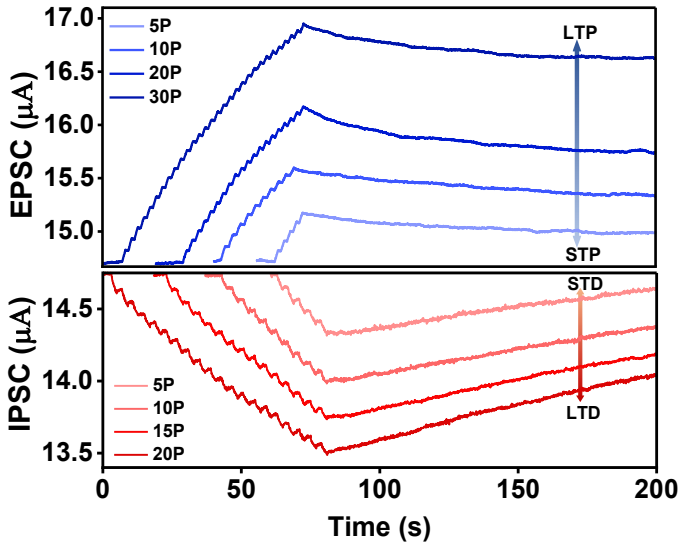


- $\text{PPF}\ (\%) = \frac{A_2}{A_1} \times 100 = C_1 e^{-\frac{t}{\tau_1}} + C_2 e^{-\frac{t}{\tau_2}} + C_3$

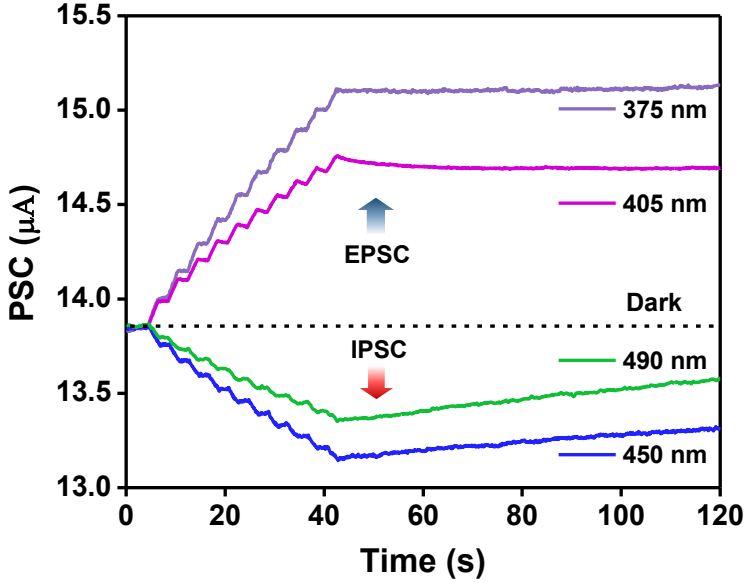
A_1 is post-synaptic response due to the first spike and A_2 due to the second spike, τ_1 and τ_2 are characteristic time constants.

- Highest PPF index is 197.6% and highest PPD index 181.4% for 500 ms interval.

Spike Number-Dependent Plasticity



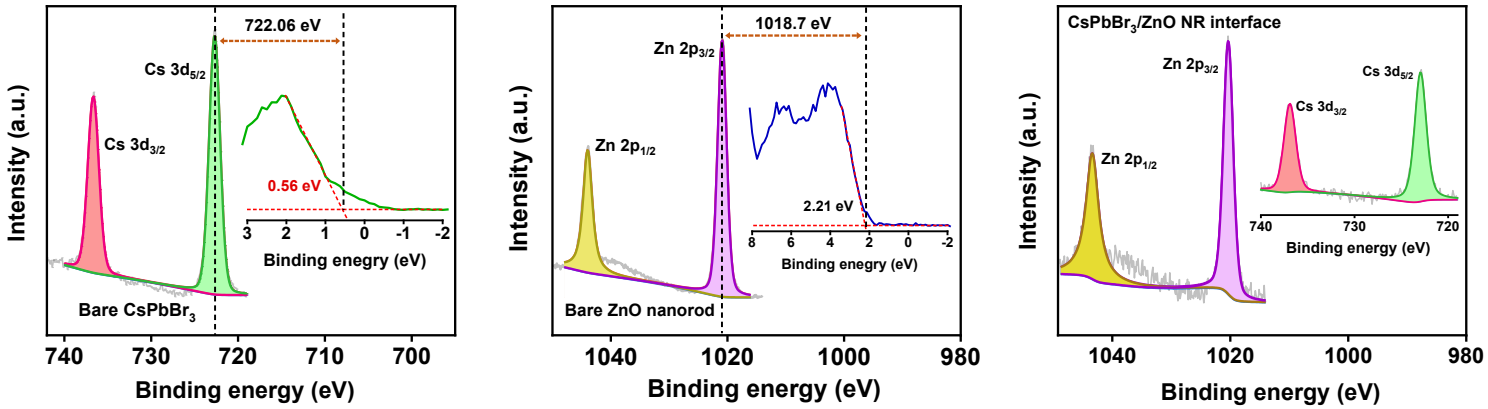
Wavelength-Dependent Plasticity

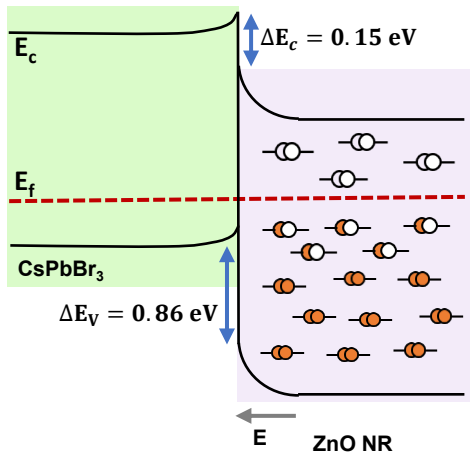


- Both excitatory and inhibitory response strength increase with number of spikes : a transition from short-term memory (STM) to long-term memory (LTM)
- Exhibits an excitatory response under 375 nm and 405 nm excitation and inhibitory responses for both 450 nm and 490 nm illumination
- Energy consumption (E) per spiking event ~ 72.5 nJ using E = V.I.t, V is the read voltage, t the optical pulse width, and I is the triggered current

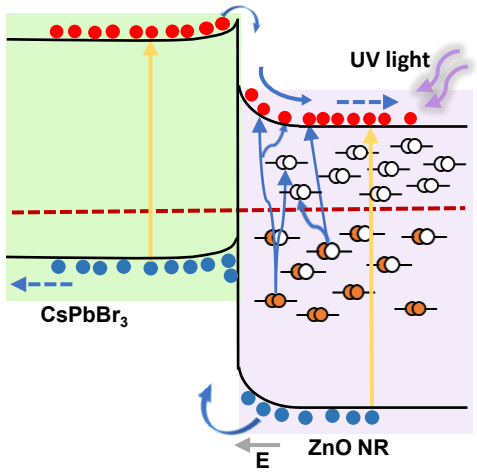
Communicated..

Mechanism for bidirectional photoresponse

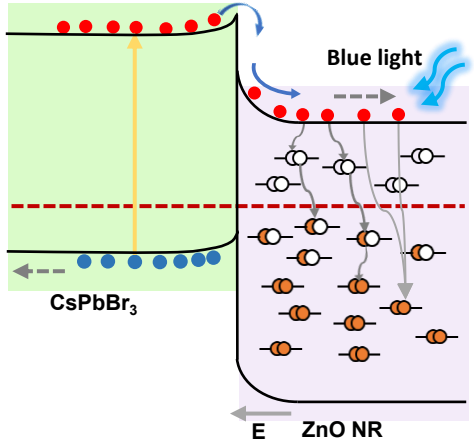




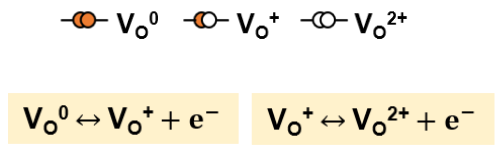
After contact



Under UV illumination

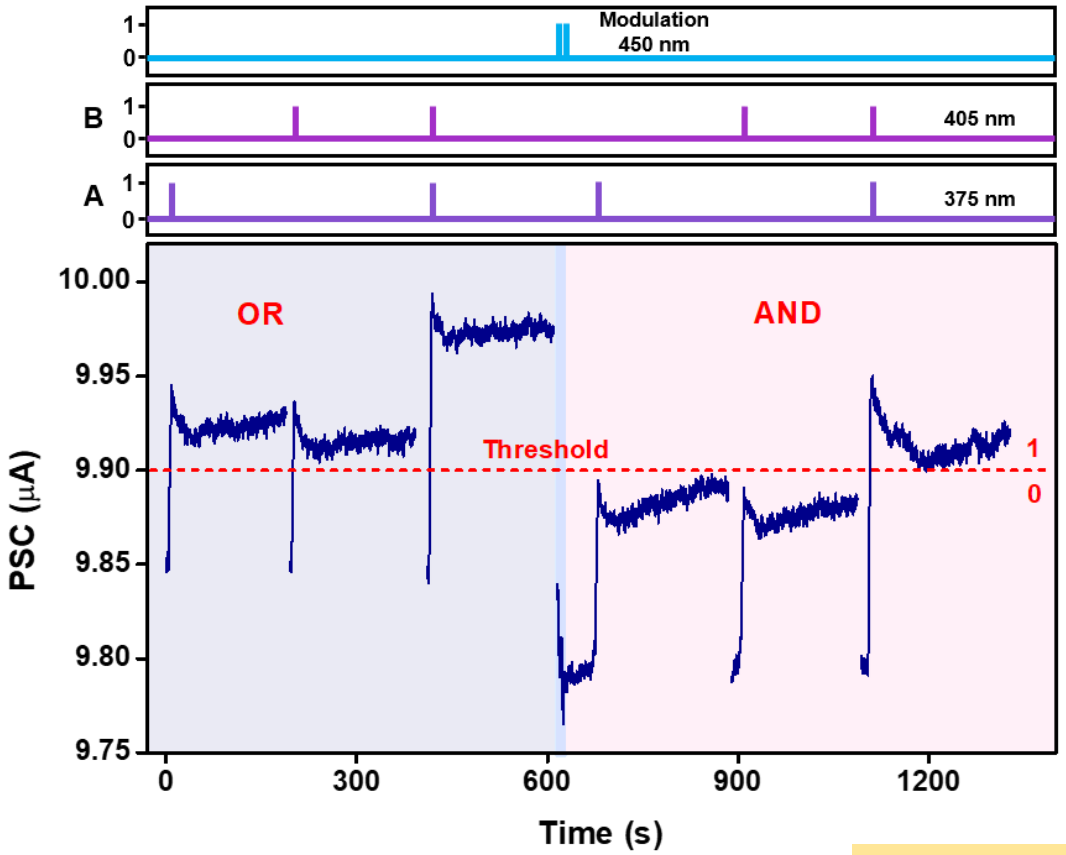


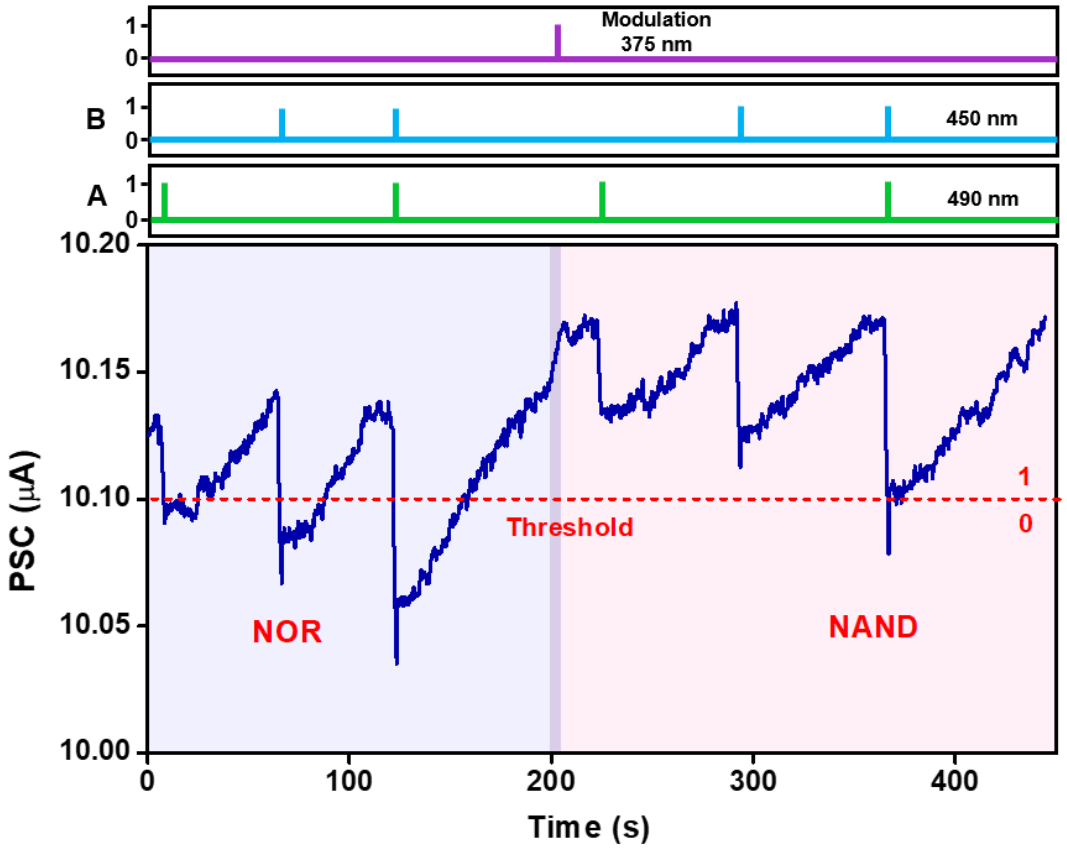
Under blue illumination



- Upon UV (375 nm) excitation, photoionization of insulating α-type ground-state oxygen vacancies (V_o) forms metastable conducting β-type doubly-ionized oxygen vacancies (V_o^{2+}), releasing electrons – leading to PPC.
- Upon Blue light excitation (450 nm), electron-hole pairs generated primarily in CsPbBr3 are captured by the doubly ionized oxygen vacancies and are deionized and return to the ground state, reducing effective charge carriers, leading to NPC effect.

Optical Logic Gate using Bidirectional Photoconductance





Optical input		Logic output			
A	B	OR	AND	NOR	NAND
0	0	0	0	1	1
0	1	1	0	0	1
1	0	1	0	0	1
1	1	1	1	0	0

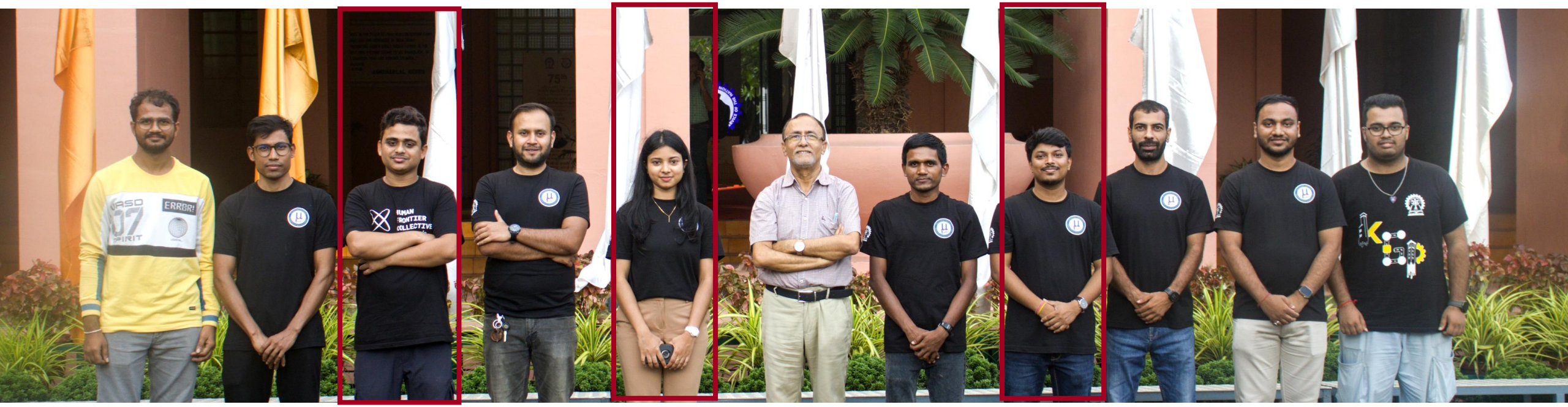
- Optical Logic gates OR, AND, NOR, and NAND implemented using the bidirectional photo response.
- To realize OR and AND Logic, 375 nm and 405 nm pulses were used as inputs, and 450 nm light was used for modulation.
- To realize NOR and NAND Logic, 375 nm and 405 nm pulses were used as inputs, and 450 nm light was used for modulation.
- Switched from OR to AND (NPC) and NOR to NAND (PPC) : modulation signal

Communicated..

Conclusion

- Heterogeneous integration : 2D WS2 & CsPbI3 – High performance phototransistor
- Demonstrated moderate efficiency CsPbI3 nanocrystals sensitized solar cells
- Engineered R-P faults in MHP : Tunable & Improved LEDs
- Optoelectronic Synapses – interface engineering to demonstrate both NPC & PPC using same material platform. Artificial vision systems, switchable optical logic gates with PPC & NPC

Acknowledgements



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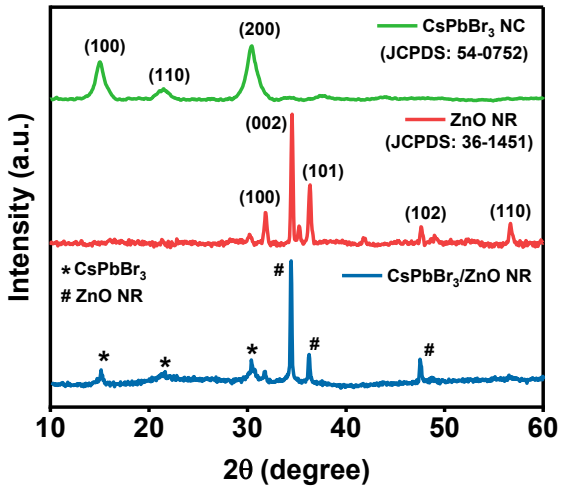
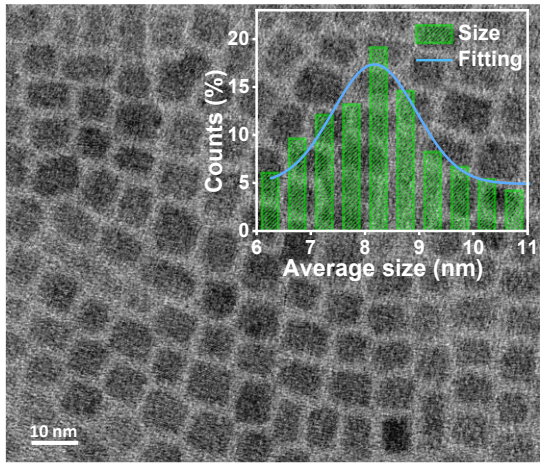
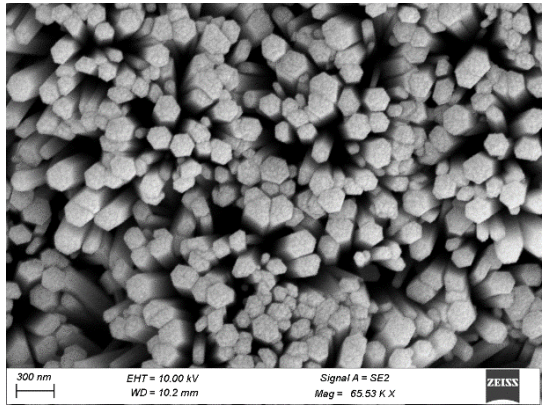
Shreyasi Das, ISTA, Austria

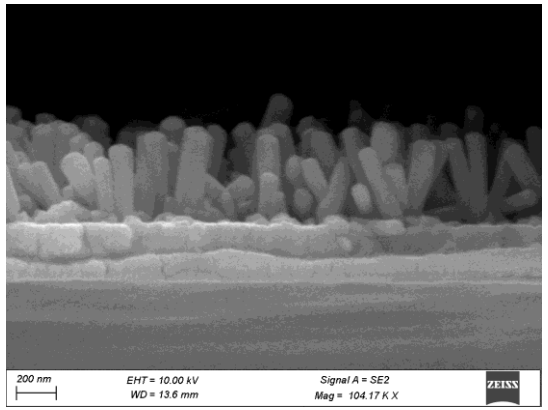
Perovskite-Oxide Heterojunction for All-Optical Synapse

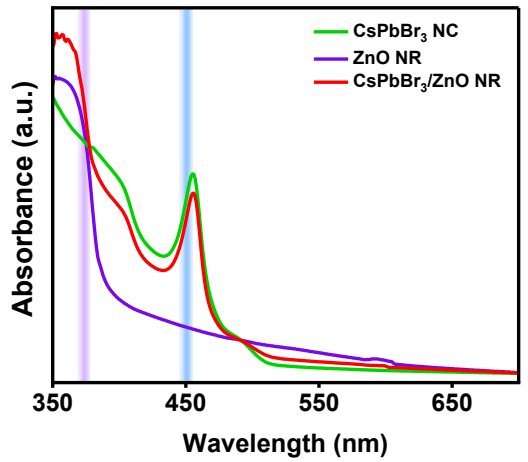
Materials Characterization

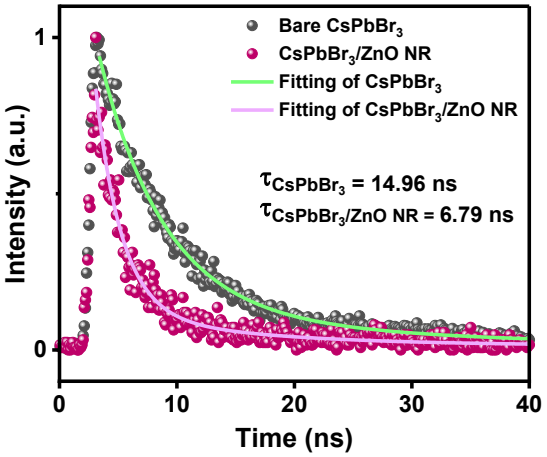


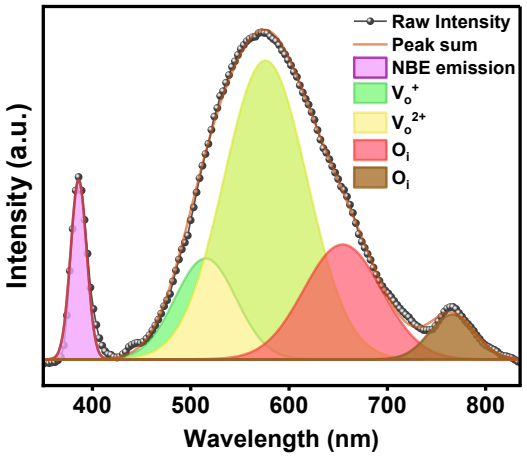


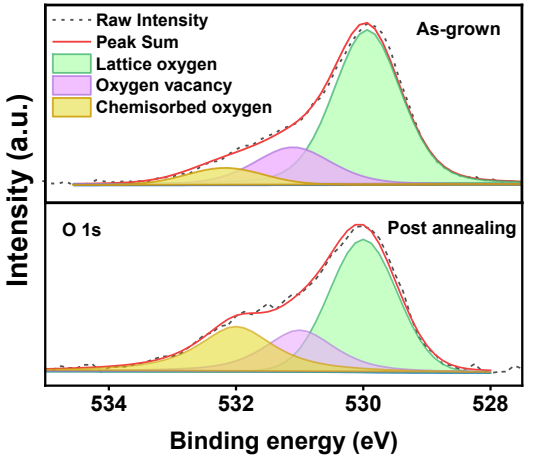












- XRD pattern reveals cubic phase of $CsPbBr_3$ nanocrystals and hexagonal wurtzite phase of ZnO with the nanorods being oriented along the c-axis.
- The average size of the synthesized $CsPbBr_3$ nanocrystals are ~ 8 ± 1 nm.
- Average length of ZnO nanorods ~450 nm and average diameter ~ 150 nm, calculated from the FESEM images.

- UV-Vis absorption spectra reveal a bandgap of 2.47 eV for $CsPbBr_3$, 3.2 eV for ZnO nanorods.
- ZnO nanorod room temperature PL spectra reveal different defect peaks (V_o, O_i).
- XPS spectra reveal that ambient annealing reduces the oxygen vacancy concentration and increases the chemisorbed oxygen content.