

In this process, alcohols serve as both aldehyde precursors and hydrogen sources. The perovskite QDs, known for their low cost, ease of processing, air stability, and tunable band edges, offer promising potential in organic transformations. Furthermore, selectivity can be easily modulated by adjusting the cocatalyst's electronic structure.

Chapter 4: In this chapter, we developed the Z-scheme heterojunction of BiOBr nanosheets and CsPbBr₃ QDs for the selective semidehydrogenation of tetrahydroisoquinoline (THIQ) to dihydroisoquinoline (DHIQ). Charge separation is driven by interfacial electric fields, with electrons transferring from BiOBr's CB to CsPbBr₃'s VB. The negative CB of CsPbBr₃ activates the molecular oxygen (O₂), forming reactive oxygen species. Optimal loading of CsPbBr₃ on BiOBr (20 wt%, Z-20) achieved a 97% yield and controlled the two-electron process for selective semidehydrogenation of THIQ to DHIQ. Transient absorption studies revealed efficient exciton dynamics, contributing to enhanced catalytic performance.

Chapter 5: In the fifth chapter, we report the modulation of lead-free metal halide perovskite (Cs₂CuBr₄) band structures by tuning synthesis methods. Photocatalyst PC-1, synthesized via hot injection, features a more negative conduction band minima (CBM) than PC-2, synthesized at room temperature, enabling more efficient O₂ activation and radical-mediated alcohol dehydrogenation. PC-1 also exhibits a more positive valence band maxima (VBM), facilitating amine oxidation: enhanced charge separation and reduced recombination further boost photocatalytic performance. PC-1 achieved up to 98% yield in the oxidative amidation of alcohols and is recyclable for over five cycles.

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List of Publications

- (i) Deciphering charge transfer dynamics of a lead halide perovskite–nickel (II) complex for visible light photoredox C–N coupling, **V. Kumar**, S. K. Patel, V. Vyas, D. Kumar, E. S. S. Iyer, and A. Indra, *Chem. Sci.*, 2024, **15**, 13218-13226.
- (ii) Visible light-driven molecular oxygen activation for oxidative amidation of alcohols using lead-free metal halide perovskite, **V. Kumar**, V. Vyas, D. Kumar, A.K. Kushwaha, E. S. S. Iyer, and A. Indra, *Chem. Sci.*, 2024, **15**, 5448-15455.
- (iii) Ligand-induced surface modification of cuprous oxide improves C₂₊ product selectivity in electrochemical CO₂ reduction, **V. Kumar**, Y. Li, A. D. Chowdhury, and A. Indra, *Mater. Today Chem.*, 2024, **41**, 102319.
- (iv) The low loading of metal in metal–organic framework-derived NiN_x@NC promotes amide formation through C–N coupling, V. Vyas, **V. Kumar** and A. Indra, *Chem. Commun.*, 2024, **60**, 2544-2547.
- (v) Halide perovskite-cobalt(III) complex photoredox catalyst for highly efficient N-Alkylation of amines with alcohols, **V. Kumar**, and A. Indra (*Submitted*).
- (vi) Z-Scheme BiOBr/CsPbBr₃ heterojunction for selective semihydrogenation of 1,2,3,4-tetrahydroisoquinoline to 3,4-dihydroisoquinoline, **V. Kumar**, S. K. Patel, S. Dhingra, D. Kumar, V. Vyas, K. Kailasam, E. S. S. Iyer, and A. Indra, (*Submitted*).
- (vii) Ultrathin Bismuthene Nanosheets with Edge-Rich Coordinative Unsaturation Promote Photocatalytic Arylation of Heteroarenes, Ajit Kumar Singh, Sandeep Patel, Sunil Patel, Akshay Kumar Mandhotra, Anjali Verma, **V. Kumar**, Kamalakannan Kailasam, E. Siva Subramaniam Iyer, Indranil Chatterjee, Arindam Indra (*Submitted*).
- (viii) Cr-induced electronic structure modulation of CoOOH for improved alcohol oxidation reactions, **V. Kumar**, Arindam Indra (*Unpublished*).
- (ix) Z-Scheme CsPbBr₃/CeO₂ Heterojunction Enhances Charge Separation for Selective sp³ C–H Activation of Toluene under Visible-Light Irradiation, **V. Kumar**, S. Kumar Patel, E. Siva Subramaniam Iyer, and Arindam Indra (*Unpublished*).