MAIN PUBLICATIONS ON PHOTOCATALYTIC WATER SPLITTING

1) Charge Localization in Defective BiVO4

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The Journal of Physical Chemistry C 126 (6), 2960-2970

2) Water‐Stable DMASnBr3 Lead‐Free Perovskite for Effective Solar‐Driven Photocatalysis

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3) Evaluation of photocatalysts for water splitting through combined analysis of surface coverage and energy-level alignment

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4) Strong Hole Trapping Due to Oxygen Dimers in BiVO4: Effect on the Water Oxidation Reaction

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5) Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water

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6) Effect of the Solvent on the Oxygen Evolution Reaction at the TiO2–Water Interface

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7) Role of Polarons in Water Splitting: The Case of BiVO4

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8) Surface polarons reducing overpotentials in the oxygen evolution reaction

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9) pH-Dependent Catalytic Reaction Pathway for Water Splitting at the BiVO4–Water Interface from the Band Alignment

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12) Comprehensive modeling of the band gap and absorption spectrum of BiVO4

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13) Experimental Strategy and Mechanistic View to Boost the Photocatalytic Activity of Cs3Bi2Br9 Lead‐Free Perovskite Derivative by g‐C3N4 Composite Engineering

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