Rational Design and Preparation of S-Scheme Heterojunction Photocatalysts for Photocatalytic Hydrogen Production

Şevval Yıldız[a]*, Yigit Osman Akyıldız[b, c]*, Emre Aslan[c], İmren Hatay Patır[a]

[a] Selcuk University, Department of Biotechnology, 42030, Konya, Türkiye e-mail: sevvl42yldz@gmail.com

[b] YEO Technology R&D Center, 34870, İstanbul, Türkiye

[c] Selcuk University, Department of Biochemistry, 42030, Konya, Türkiye

The growing global energy demand, fossil-fuel depletion, and environmental concerns have intensified the need for sustainable energy technologies. Hydrogen is a promising clean energy carrier due to its high energy density and potential to reduce carbon emissions. For sustainable hydrogen production, developing efficient photocatalysts to directly convert solar energy into chemical energy is crucial. Two-dimensional (2D) semiconductor catalysts exhibit enhanced performance compared to bulk counterparts due to their large specific surface areas and abundant active edge sites. Among these, Group 15 2D pnictogens have attracted substantial attention in photocatalytic energy conversion due to their distinctive electronic properties. However, limited light absorption, rapid photogenerated electron–hole recombination, and inefficient charge transfer restrict photocatalytic hydrogen production efficiency. S-scheme heterojunctions enhance performance by improving light absorption and promoting efficient charge-carrier separation. $BiVO_3$ is an important photocatalyst with strong oxidation capability arising from its favorable band structure. Herein, an S-scheme phosphorene/$BiVO_3$ heterojunction was constructed by coupling 2D phosphorene with $BiVO_3$ prepared via liquid-phase self-assembly. This heterojunction was characterized by structural, morphological, and optical techniques. An internal electric field effectively suppressed charge carrier recombination while preserving phosphorene's strong reduction capability and $BiVO_3$'s oxidation capability, enhancing overall photocatalytic activity. To optimize performance, S-scheme $BiVO_3$/phosphorene heterojunctions with phosphorene loading ratios of 25%, 50%, and 75% were synthesized and their hydrogen evolution systematically compared. The 75% phosphorene heterojunction exhibited the highest photocatalytic hydrogen production after an eight-hour reaction. These findings demonstrate the developed heterojunction is a promising photocatalyst for solar-driven hydrogen production.

Keywords: Hydrogen production, photocatalysis, pnictogens, S-scheme,

Acknowledgment: This project is financially supported by TUBITAK-1001 programme (Grant number: 123Z412).