Defect Engineering Strategy to Enhance Hydrogen Performance of ZnO/CdS Photocatalysts

Yeongsu Choi, Hyemin Park, Hanju Lee, Junghyeun Kim*

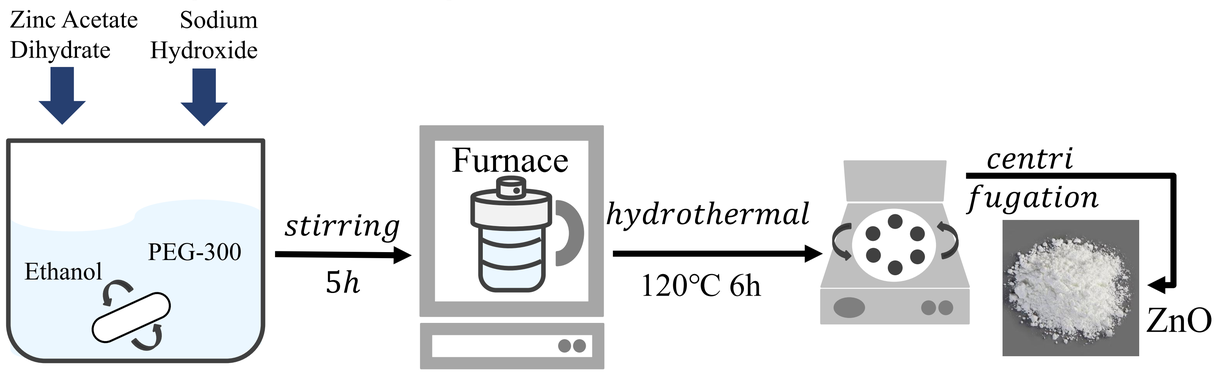
Department of Chemical Engineering, University of Seoul, Seoul, Korea

Abstract

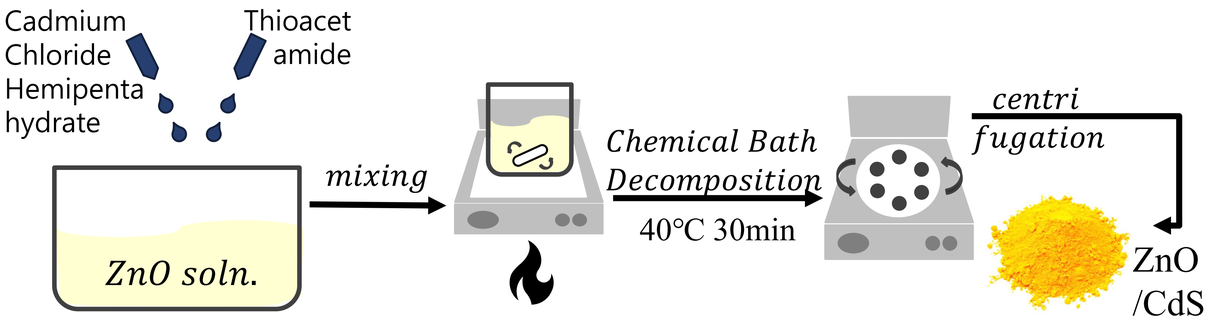
Photocatalytic hydrogen production is a promising strategy for carbon-neutral energy conversion; however, its efficiency is limited by rapid charge recombination and poor visible-light utilization. Herein, a ZnO/CdS heterojunction photocatalyst with Cd-defect-rich CdS was designed through sulfur-rich synthesis conditions to enhance photocatalytic hydrogen evolution. The introduced Cd defects regulate the electronic structure and promote charge separation, while the ZnO/CdS direct Z-scheme heterojunction facilitates efficient interfacial charge transfer and improves photocatalytic stability. As a result, the defect-engineered ZnO/CdS photocatalyst exhibited enhanced photocatalytic hydrogen-production performance under visible-light irradiation.

Experimental

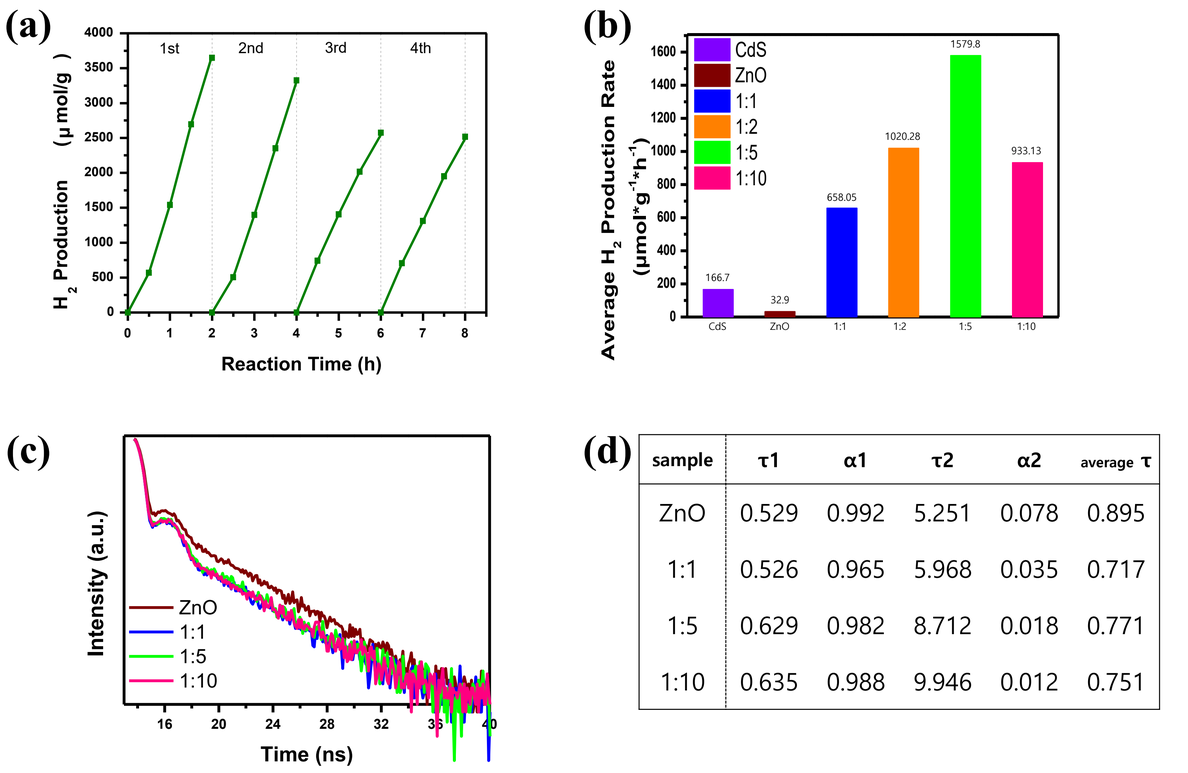
◆ ZnO Synthesis via Hydrothermal Method



◆ ZnO/CdS Synthesis via Chemical Deposition Method



Results & Discussion



(d)

sample	τ1	α1	τ2	α2	average τ
ZnO	0.529	0.992	5.251	0.078	0.895
1:1	0.526	0.965	5.968	0.035	0.717
1:5	0.629	0.982	8.712	0.018	0.771
1:10	0.635	0.988	9.946	0.012	0.751

Figure 1. (a) Stability Evaluation of Photocatalytic Hydrogen Production over ZnO/CdS(1:5) photocatalysts (b) Comparison of Average Hydrogen Production Rates (c) & (d) Time-Resolved Photoluminescence (TRPL) Decay Curves and fitted lifetime parameters of ZnO/CdS Photocatalysts

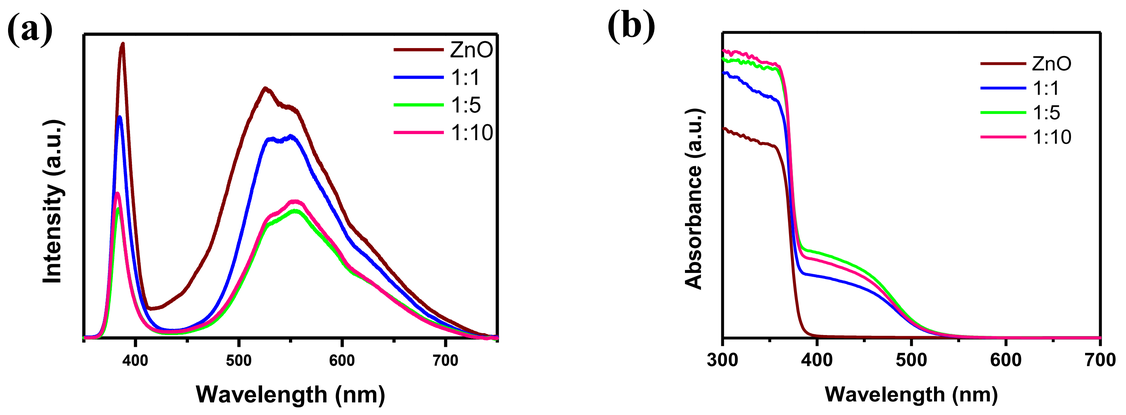


Figure 2. (a) Raman Spectra of ZnO/CdS Photocatalysts with Different Cd:S Ratios, (b) UV–Vis Diffuse Reflectance Spectra (DRS) of ZnO/CdS Photocatalysts with different Cd:S ratios

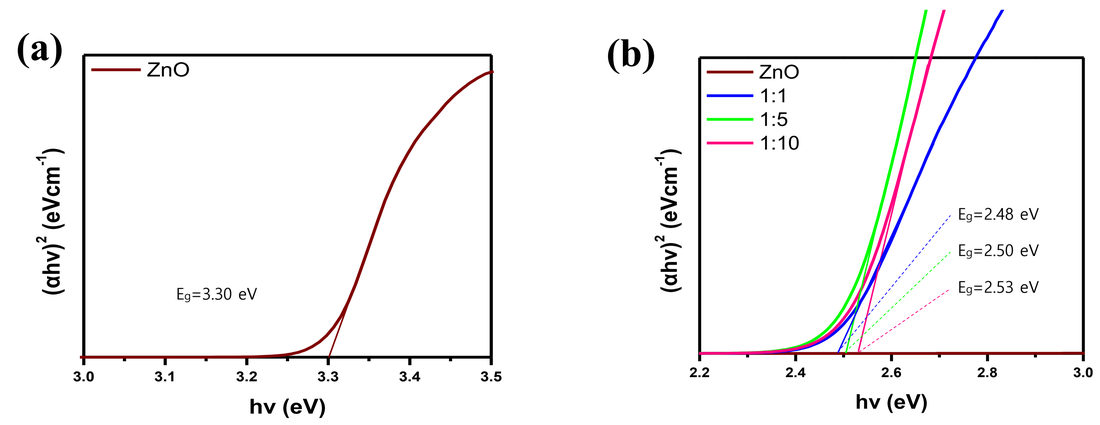


Figure 3. (a) & (b) Tauc plots and bandgap energies of ZnO and ZnO/CdS photocatalysts

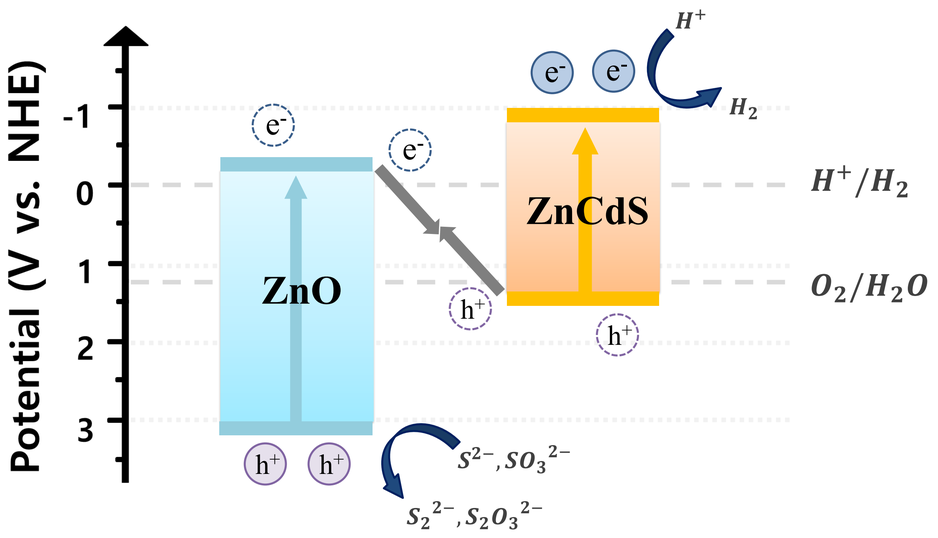


Figure 4. Schematic diagram of a Z-scheme charge transfer pathway, and hydrogen production mechanism over the ZnO/ZnCdS photocatalyst

Summary

- ZnO/CdS photocatalysts with Cd defects were synthesized under sulfur-rich conditions by controlling the Cd:S ratio. Among the tested ratios (1:1, 1:2, 1:5, and 1:10), the 1:5 sample exhibited the highest photocatalytic H_2-production activity.
- Increasing the sulfur content promoted Cd-defect formation and improved photocatalytic performance; however, excessive sulfur introduction led to performance deterioration due to increased charge recombination.
- The optimal ZnO/ZnCdS (1:5) sample showed enhanced H_2 evolution by promoting charge separation and interfacial charge transfer while maintaining the favorable direct Z-scheme heterojunction structure.

Reference

1) Wang, Sheng, et al. "Direct Z-scheme ZnO/CdS hierarchical photocatalyst for enhanced photocatalytic H_2-production activity." Applied Catalysis B: Environmental 243 (2019): 19-26.
2) Enhanced photocatalytic H2 production of CdS by the introduction of Cd vacancies Bihan Li. Chem. Commun., 2025, 61, 15630–15633
3) ZnO/ZnS/CdS three-phase composite photocatalyst with a flower cluster structure : Research on its preparation and photocatalytic activity hydrogen production. Kai He. Volume 51, Part B, 2 January 2024, 30-40

Nano System Applications Laboratory