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Tunable Band Gaps and Conduction Band Edges of CdS/ZnS Heterostructures – A First-Principles-Based Prediction

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The density of states for the $Cd_{0.5}Zn_{0.5}S$ solid solution was calculated to further investigate the differences between the solid solution effect and the covalent heterostructure effect on improved photocatalytic performance. The structural model for the $Cd_{0.5}Zn_{0.5}S$ solid solution was constructed using the special quasi-random structure (SQS) approach. Our calculations reveal that the band gap for the $Cd_{0.5}Zn_{0.5}S$ solid solution is 2.68 eV (Figure S1), which is significantly larger than the 2.07 eV observed for the $(CdS)_5/(ZnS)_5$ heterostructure. The reduced band gap in the CdS-ZnS heterostructure naturally leads to enhanced photocatalytic performance. These findings indicate that, for the CdS-ZnS system, the covalent heterostructure effect plays a more significant role in improving photocatalytic performance compared to the solid solution effect.

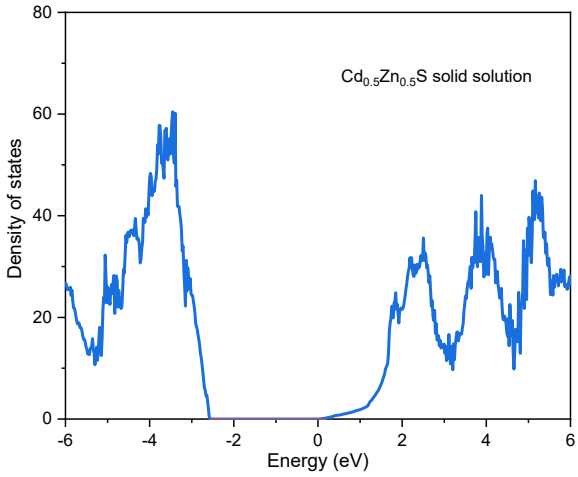

Figure S1. Density of states for a $Cd_{0.5}Zn_{0.5}S$ solid solution.