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Synthesis of Highly Active Octahedral $NaInS_2$ for Enhanced H_2 Evolution

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Abstract : Crystal facet engineering, which involves tuning and controlling a crystal surface and morphology, is a commonly employed strategy to optimize the performance of crystalline nanocrystals. The principle behind this strategy is that surface atomic rearrangement and coordination, which inherently determines their catalytic activity, can be easily tuned by morphological control. Because of this, the catalytic properties of a nanocrystal are closely related to the surface of an exposed facet, and it has provided great motivation for researchers to synthesize photocatalysts with high catalytic activity by maximizing reactive facets exposed through morphological control. In this contribution, octahedral $NaInS_2$ crystals have been successfully developed via solvothermal method. The formation of the octahedral $NaInS_2$ crystals was investigated using field emission scanning electron microscope (FESEM) and X-Ray diffraction (XRD), and results have shown that the concentration of sulphur precursor plays an important role in the growth process, leading to the formation of other $NaInS_2$ crystal structures in the form of hexagonal nanosheets and microspheres. Structural modeling analysis suggests that the octahedral $NaInS_2$ crystals were enclosed with {012} and {001} facets, while the nanosheets and microspheres are bounded with {001} facets only and without any specific facets, respectively. Visible-light photocatalytic H_2 evolution results revealed that the octahedral $NaInS_2$ crystals (~67 μmol/g/hr) exhibit ~6.1 and ~2.3 times enhancement as compared to the conventional $NaInS_2$ microspheres (~11 μmol/g/hr) and nanosheets (~29 μmol/g/hr), respectively. The H_2 enhancement of the $NaInS_2$ octahedral crystal is attributed to the presence of {012} facets on the surface. Detailed analysis of the octahedron model revealed obvious differences in the atomic arrangement between the {001} and {012} facets and this can affect the interaction between the water molecules and the surface facets before reducing into H_2 gas. These results highlight the importance of tailoring crystal morphology with highly reactive facets in improving photocatalytic properties.

Keywords : H_2 evolution, photocatalysis, octahedral, reactive facets
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