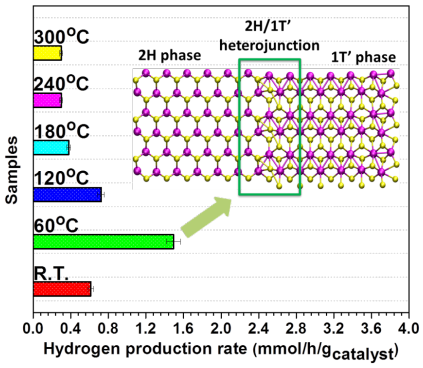
Multiphase MoS_2 Monolayers as Efficient Photocatalysts for Hydrogen Production from Water Splitting

Achievement: 2D multiphasic MoS_2 nanosheets were synthesized and tailored as visible light photocatalysts for efficient solar hydrogen production from water splitting.

Significance and Impact: Development of efficient and inexpensive photocatalysts that don't involve noble metals is crucial for harvesting solar energy into fuels.



Multiphasic MoS_2 treated at 60°C synergizes the photocatalyst (2H) and co-catalyst (1T') and enhances the photocatalytic solar hydrogen production.

Research Details:

- A chemical exfoliation method was developed to produce single layer multiphasic MoS_2
- The content of each phase (2H,1T, 1T') of MoS_2 was tuned by varying the annealing temperature
- DFT calculations correlated the 2H/1T' heterojunctions to the efficient separation of photogenerated charge carriers and abundant active basal sites for hydrogen evolution in addition to the edge sites

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Overview:

This work shows how the confluence of unique optical, electronic and chemical properties of 2D MoS_2 monolayers can be fully captured for efficient photocatalytic water splitting. 2D single-layer MoS_2 nanosheets are demonstrated as efficient photocatalysts for hydrogen evolution reaction (HER) from water splitting thanks to specific in-plane heterojunctions constructed in the MoS_2 monolayer. These functional heterojunctions are formed among the different phases of chemically exfoliated MoS_2 monolayers: semiconducting 2H, metallic 1T, and nearly-metallic 1T' phases. The proportion of the three MoS_2 phases can be systematically controlled via thermal annealing of the nanosheets. Interestingly, a volcano relationship is observed between the photocatalytic HER activity and the annealing temperature with an optimum activity obtained after annealing at 60ºC. The presence of 2H/1T' heterostructures in the 60 °C treated MoS2 is responsible for the efficient separation of photogenerated charge carriers and abundant active basal sites for hydrogen evolution, as supported by results from Raman, XPS, conductive AFM,

time-resolved spectroscopy, and the plane-wave DFT calculations. It clearly demonstrated that MoS_2 nanosheets can be rationally engineered via phase manipulation to enable efficient hydrogen evolution from water splitting under visible light irradiation.