2D/2D heterostructure based on borophene/ MoS_2 for photo-, electro- and photoelectro-catalytic hydrogen evolution – mechanistic insight

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The urgent need for sustainable energy solutions has driven extensive research into solar-driven hydrogen production via photoelectrochemical (PEC) processes. Molybdenum disulfide (MoS_2) has emerged as a promising catalyst due to its excellent electronic and catalytic properties. The recent discovery of borophene, a new two-dimensional (2D) boron-based material with remarkable electronic characteristics and tunable band structures, presents a unique opportunity to enhance MoS_2-based PEC performance.

In this presentation, I will introduce the fabrication, characterization, and application of borophene/molybdenum disulfide (B/MoS_2) 2D/2D heterostructures for efficient hydrogen evolution. The study explores their catalytic performance in photo- (photo), electro- (HER), and photoelectro- (PEC) catalytic hydrogen evolution reactions under acidic conditions. Moreover, in-situ and ex-situ material characterization techniques were employed to elucidate the underlying reactions mechanisms.

Our results show that optimizing the MoS_2-to-borophene mass ratio significantly enhances PEC performance, reducing the overpotential to 281.1 mV with a Tafel slope of 56.0 mV/dec, substantially improved from 312.5 mV and 160.9 mV/dec in conventional HER. Moreover, long-term stability tests at a constant current density of 10 mA/cm^2 confirm the exceptional durability of B/MoS_2, maintaining stable hydrogen evolution performance for over 120 hours. The hydrogen evolution rate reached ~2.5 mol/g in PEC, representing a 1.4-fold, 1.8-fold, and 3152-fold increase compared to pristine MoS_2 in the photoelectro-, electro-, and photo-catalytic hydrogen evolution process, respectively. The comprehensive material characterization highlighted the potential of borophene-enriched MoS_2 as an efficient catalyst for solar and/or electricity-driven hydrogen production, confirming that borophene presence substantially promotes the 2H-to-1T phase transition of MoS_2 by creating strain and defects, destabilizing the 2H phase, and favoring the formation of the 1T phase, thus significantly enhancing catalytic performance.

This work underscores the potential of MoS_2/borophene heterostructures as next-generation catalysts for solar-driven hydrogen production. The findings provide valuable insights into designing advanced catalytic materials for clean energy applications and contribute to the broader efforts toward developing efficient and scalable PEC systems.