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First-Principles Study of 2D Materials for Photochemical/Electrochemical Applications

Based on first-principles calculation, we show that a non-Janus MoSSe/WSSe heterobilayer can be much more advantageous than Janus heterobilayer for the photocatalytic reduction of CO_2 to CO or HCOOH due to the absence of vertical polarization.[1] Also will be described is a series of recent collaborations with a sophiscated experimental group for photocatalytic/electrocatalytic water splitting and CO_2 reduction on 2D materials. First, combined experimental and theoretical effort is described for efficient photoelectrochemical water splitting of *p*-GeAs/*n*-Si and *p*-GeP/*n*-Si heterojunctions based on the band edge positions obtained from band structure calculation.[2,3] Second, our calculation on the activation barrier of Volmer-Heyrovsky reaction gives deep insight into our experimental results, which have shown that the 1T'-phase guest-intercalated MoS_2/WS_2 nanosheets synthesized by one-step hydrothermal reaction exhibit excellent catalytic activity toward hydrogen evolution reaction (HER).[4-6] Third, another calculation on the Gibbs free energy along the reaction path for Se-rich $MoSe_2$ and Ru,Co-coped MoS_2 also lead us to understand their chemical structures as well as their excellent catalytic activity toward the HER and CO_2 reduction under both acidic and basic conditions.[7,8]

References

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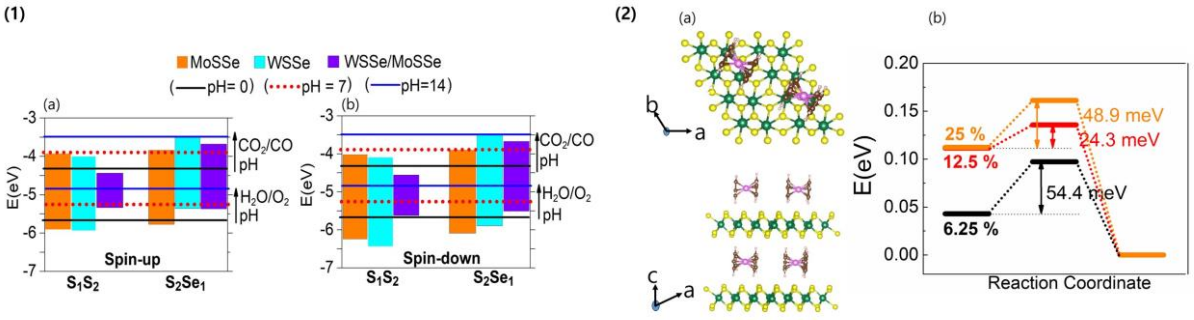

Figure 1: (a) Spin-up and (b) spin-down components of the band edge positions of the MoSSe and WSSe monolayers as well as those of the WSSe/MoSSe heterobilayer in non-Janus (S_2Se_1) and Janus (S_1S_2) configurations.
Figure 2: (a) Structure of 1T' phase (4×4) $2WS_2$-$CoCp_2$-4 (at 12.5%) in top and side views, where $CoCp_2$ is cobaltocene. (b) Comparison of the activation barrier of Heyrovsky reaction at various concentration of $CoCp_2$.