

ADVANCED FUNCTIONAL MATERIALS

Supporting Information

for *Adv. Funct. Mater.*, DOI: 10.1002/adfm.202002939

Multifunctional Lateral Transition-Metal Disulfides Heterojunctions

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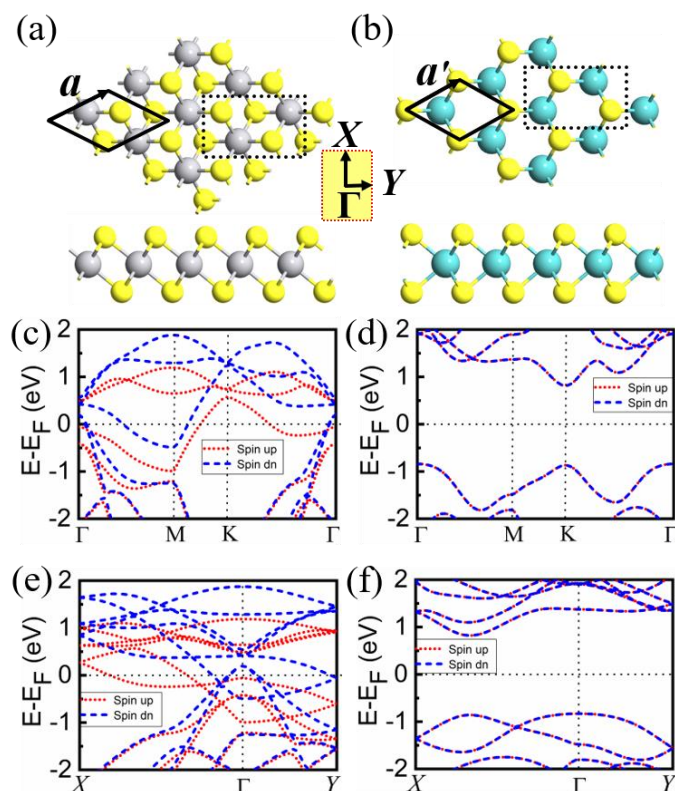


Figure S1. Schematics and spin-resolved band structures of 1T-VS₂ and 1H-MoS₂ monolayers. (a), (c), and (e) for 1T-VS₂. (b), (d), and (f) for 1H-MoS₂.

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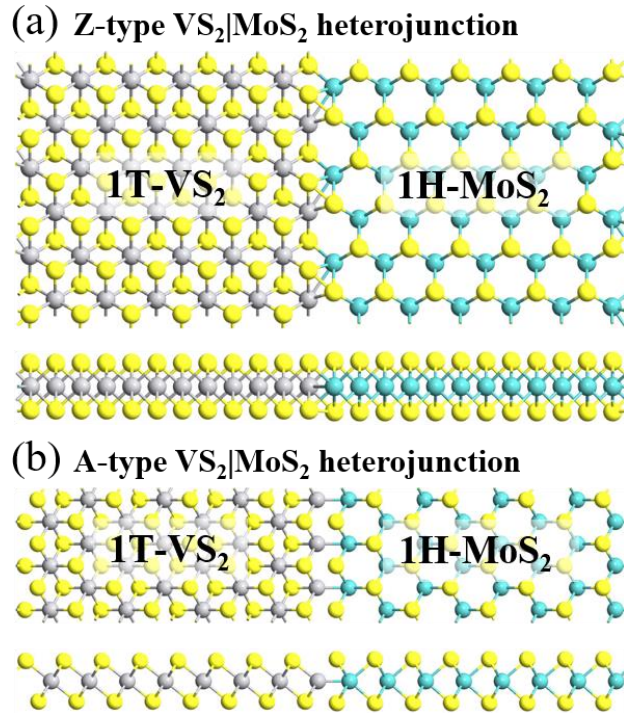


Figure S2. Schematics of two types of lateral $\text{VS}_2|\text{MoS}_2$ heterojunctions. Top (upper) and side (lower) views of (a) Z-type and (b) A-type.

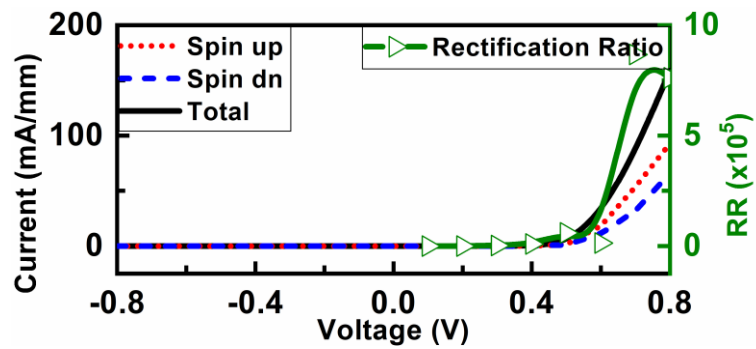


Figure S3. The I - V and rectification ratio curves of Z-type $\text{VS}_2|\text{MoS}_2$ heterojunction diode with V atom vacancy defect at the interface.

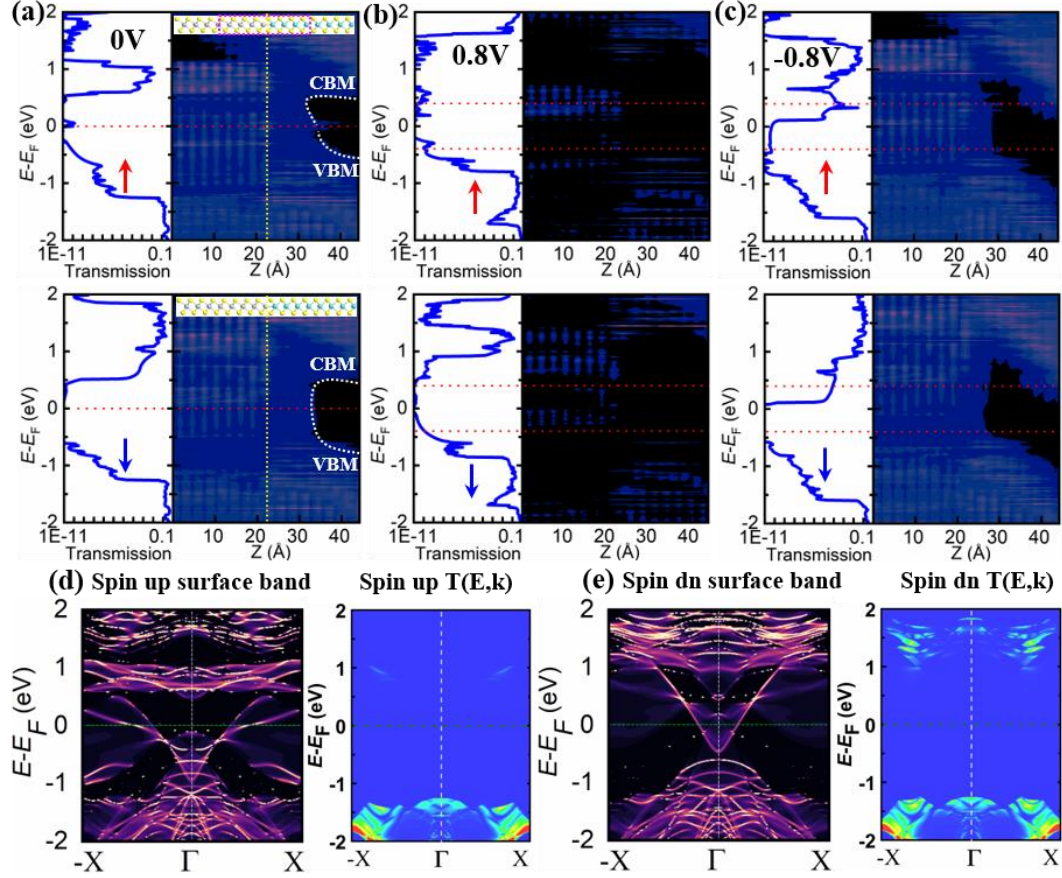


Figure S4. Projected local density of states of A-type VS₂|MoS₂ heterojunction diode at (a) 0 V, (b) 0.8 V, and (c) -0.8 V. The upper (lower) are the spin up (down) PLDOS, respectively. The Fermi level is set to zero. CBM (VBM) indicate the conduction band minimum (valence band maximum) values, respectively. Surface band of the region near the interface (see the pink rectangle of Figure S4a) and k-dependent transmission coefficients for the spin up (d) and spin down (e) states.