Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supplementary Material

Controllable Spin Rectification Behavior of Vertical and Lateral VSe_2/WSe_2 Heterojunctions Schottky Diodes

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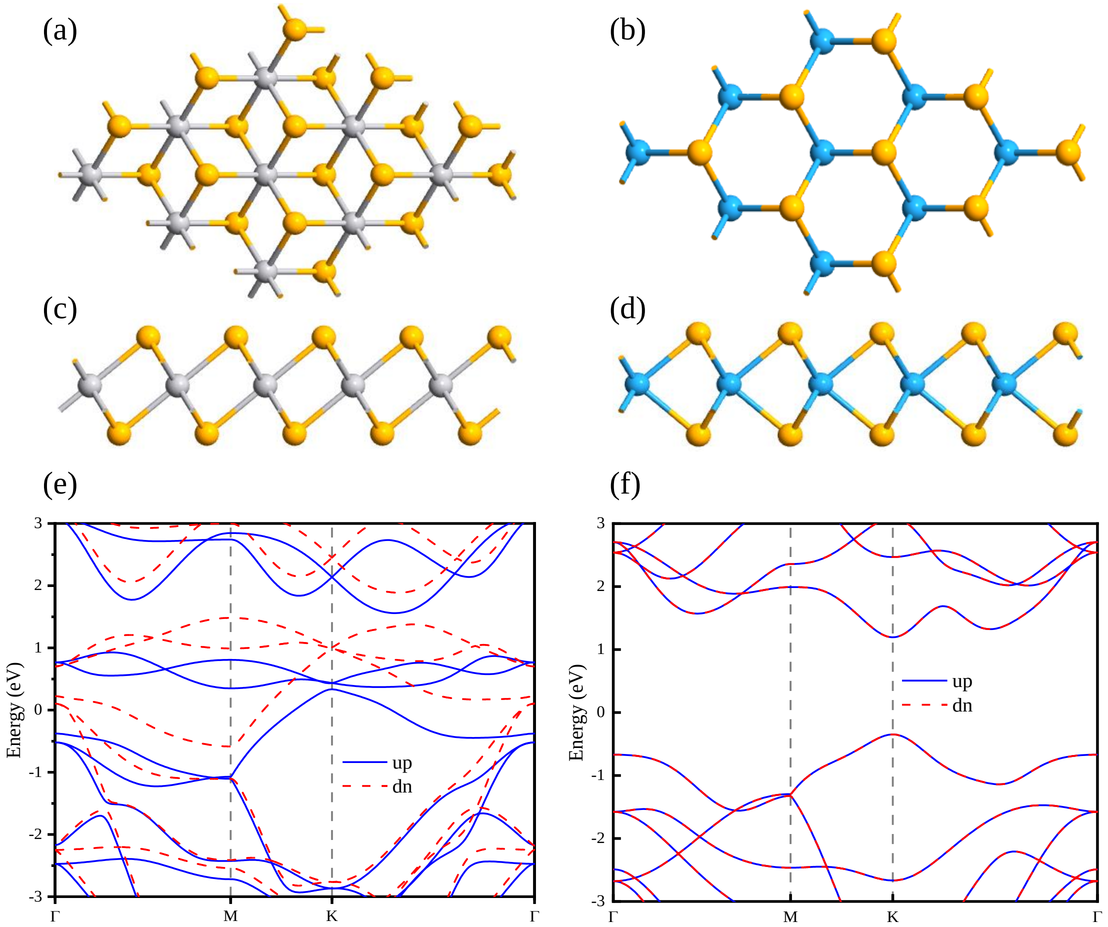

Figure S1. (a), (c), and (e): top view, side view, and band structure of 1T-VSe_2, respectively. (b), (d), and (f): top view, side view, and band structure of 2H-WSe_2, respectively.

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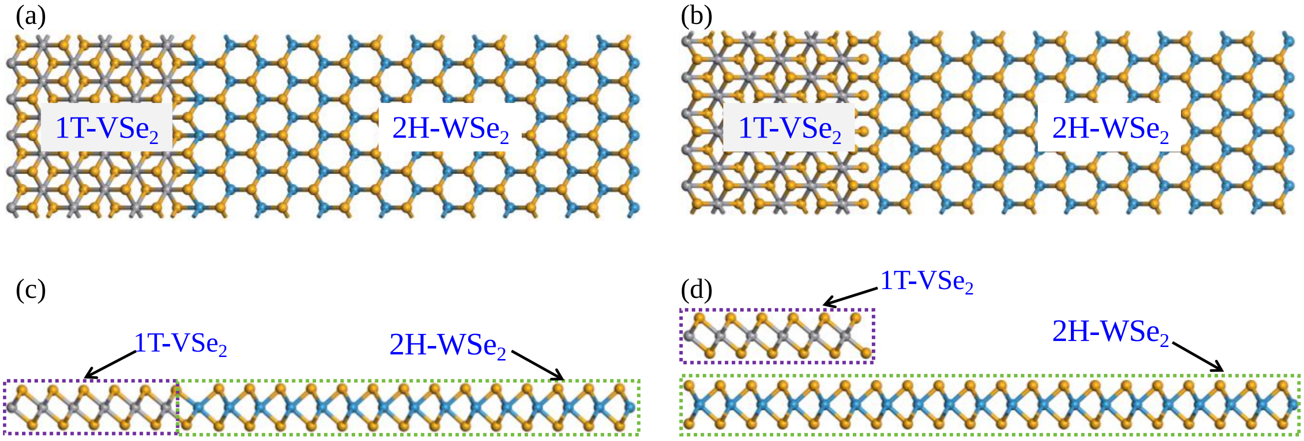

Figure S2. (a) and (c) are top and side views of the *L*-type VSe$_2$/WSe$_2$ heterojunction, respectively. (b) and (d) are top and side views of the *V*-type VSe$_2$/WSe$_2$ heterojunction, respectively.

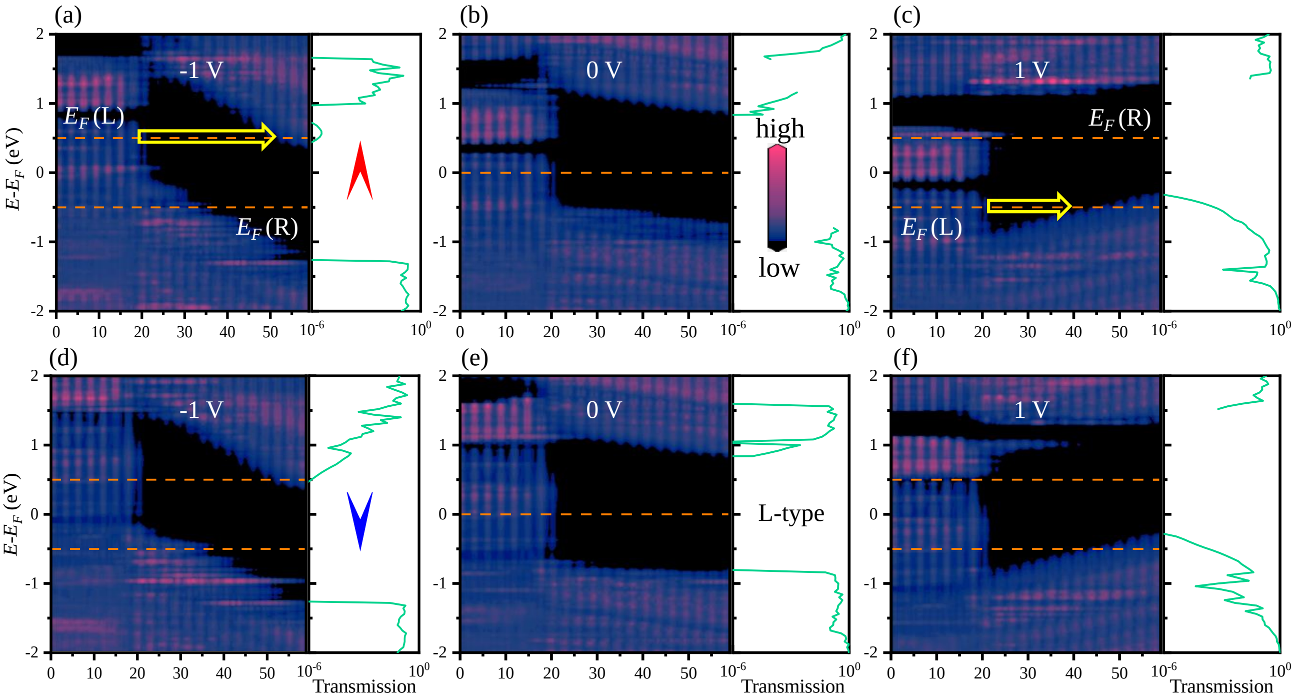

Figure S3. PLDOS (left) and transmission spectra (right) of *L*-type VSe$_2$/WSe$_2$ heterojunction Schottky diode under different biases with zero gate voltage. (a)-(c) and (d)-(f) are spin-up and spin-down states, respectively.

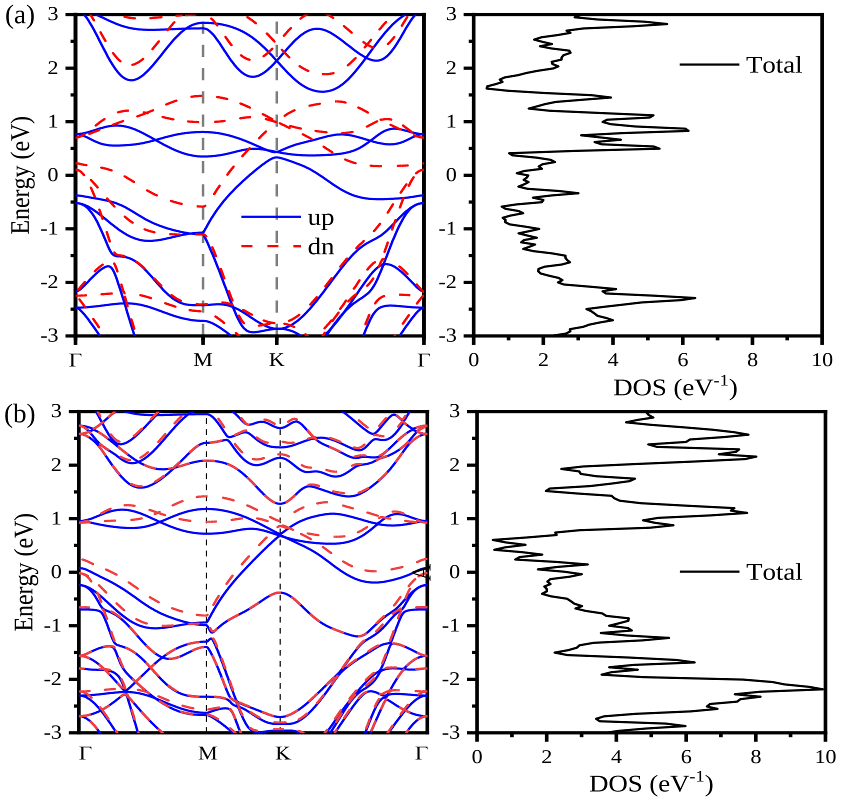

Figure S4. (a) Band structure and density of states (DOS) of 1T-VSe$_2$. (b) Band structure and DOS of the vertical heterostructure (1T-VSe$_2$ and 2H-WSe$_2$).

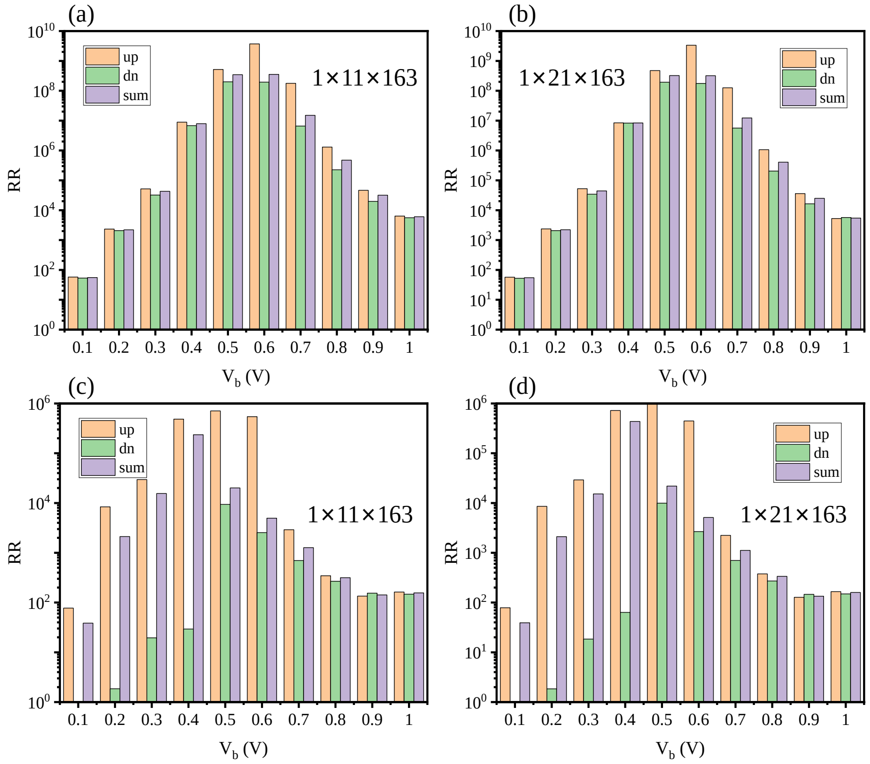

Figure S5. (a) and (b) Rectification ratios of the vertical VSe$_2$/WSe$_2$ heterojunction diode at 1 × 11 × 163 and 1 × 21 × 163 *k*-point grids. (c) and (d) Rectification ratios of the lateral VSe$_2$/WSe$_2$ heterojunction diode at different *k*-point grids.

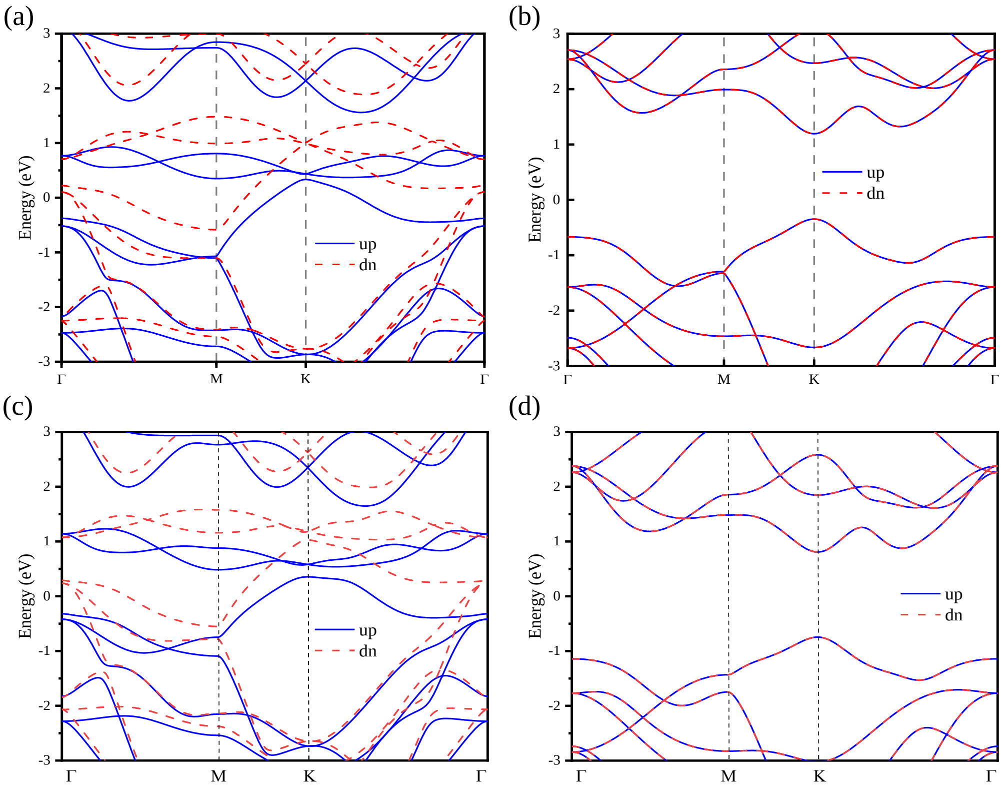

Figure S6. Band structures calculated using the VASP software package: (a) 1T-VSe_2 and (b) 2H-WSe_2. Band structures calculated using the QuantumWise ATK software package: (c) 1T-VSe_2 and (d) 2H-WSe_2.

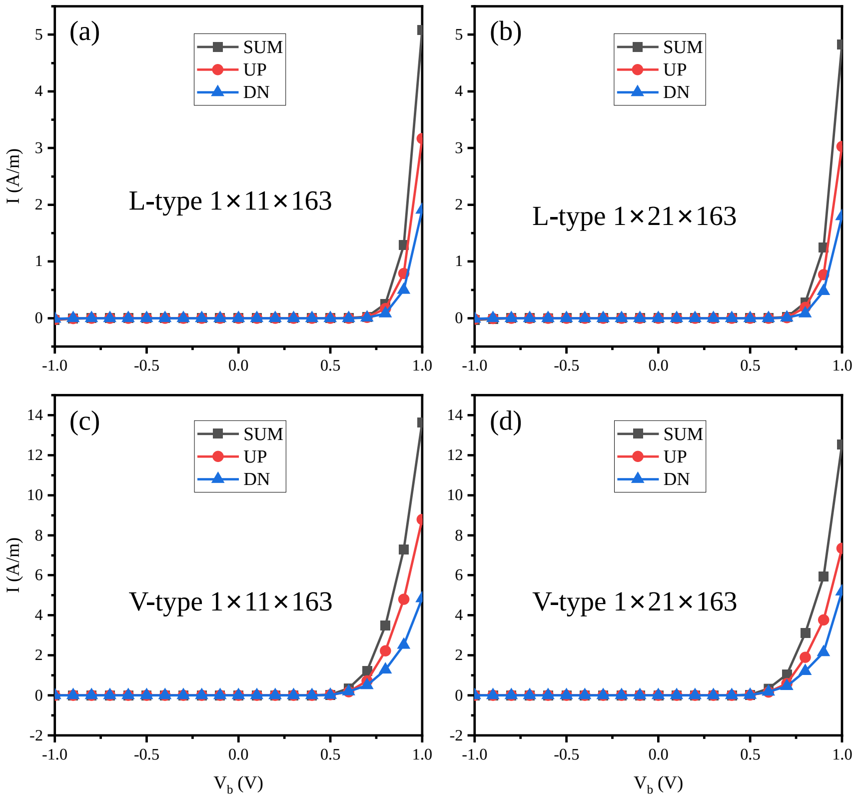

Figure S7. (a) and (b) *I-V* curves of the lateral VSe_2/WSe_2 heterojunction diode at 1 × 11 × 163 and 1 × 21 × 163 *k*-point grids. (c) and (d) *I-V* curves of the vertical VSe_2/WSe_2 heterojunction diode at different *k*-point grids.