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Supplementary Information

Tunable Schottky contacts in MoSe₂/NbSe₂ (M = Mo, W) heterostructures and

promising application potential in field-effect transistors

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Fig. S1 Atomic models of the $MSe_2/NbSe_2$ (M = Mo or W) heterobilayers and their relative energies with four different types of stacking: (a) AA, (b) C1, (c) AB, and (d) C2. *d* denotes the interlayer distance between top-layer Se and lower-layer Se atoms.



Fig. S2 Band structures of (a) MoSe₂/NbSe₂ and (b) WSe₂/NbSe₂ heterobilayers by PBE functional, and the Schottky barriers Φ_{Bn} and Φ_{Bp} are denoted. Superposition of the band structures of isolated monolayers of (c) MoSe₂ and NbSe₂ and (d) WSe₂ and NbSe₂. The blue and orange lines represent the contributions from MSe₂ and NbSe₂, respectively. The Fermi level is set to zero.



Fig. S3 (a) The plane-averaged charge density difference $\Delta \rho$ for the MoSe₂/NbSe₂ composite at equilibrium distance along the *Z* direction. The inset is the 3D isosurface of the charge density difference, the yellow and blue regions represent electron accumulation and depletion, respectively. (b) Evolution of transferred electrons from MoSe₂ to NbSe₂ as the function of interface distance.



Fig. S4 (a) Evolution of the band edges as a function of the external field for $WSe_2/NbSe_2$ heterobilayer. Band structures of the $WSe_2/NbSe_2$ heterobilayer under different external field of (a) E = -0.06 V/Å, (b) E = 0.0 V/Å, and (c) E = 0.12 V/Å.



Fig. S5 (a) Evolution of Schottky barriers Φ_{Bp} and Φ_{Bn} as a function of the biaxial strain in MoSe₂/NbSe₂ heterostructure. Projected DOS on Mo atoms under strain of (b) 0%, (c) 3% and (d) 6%. The projected DOS of the s and p orbitals (multiplied with 10) is enlarged to make them visible. The Fermi level is set to zero.



Fig. S6 Band structures of the $WSe_2/NbSe_2$ heterobilayer with biaxial strain of (a) – 1%, (b) 0%, (c) 1%, (d) 2% and (e) 3%. The blue, orange and red lines represent the contributions from NbSe₂, CB and VB of WSe₂, respectively. The Fermi level is set to zero.