ADVANCED MATERIALS

Supporting Information

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Selective Interfacial Excited-State Carrier Dynamics and Efficient Charge Separation in Borophene-Based Heterostructures

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Table S1. The binding energies of β_{12}, χ_3, and α' borophenes/MoS_2 and graphene/MoS_2 heterojunctions.

	β_{12}/MoS_2	χ_3/MoS_2	α'/MoS_2	graphene/MoS_2
Binding energies (eV)	–0.35	–1.00	–2.26	–2.75

Table S2. The lattice parameters for the pristine β_{12}, χ_3, and α' borophenes, MoS_2 and borophene/MoS_2 heterojunctions.

	β_{12}	χ_3	α'	MoS_2	β_{12}/MoS_2	χ_3/MoS_2	α'/MoS_2
a (Å)	2.93	2.91	5.05	3.17	3.05	3.04	9.80
b (Å)	5.07	8.40	5.05	3.17	5.28	16.63	9.80
α (°)	90	90	90	90	90	90	90
β (°)	90	90	90	90	90	90	90
γ (°)	90	90	120	120	90	90	120

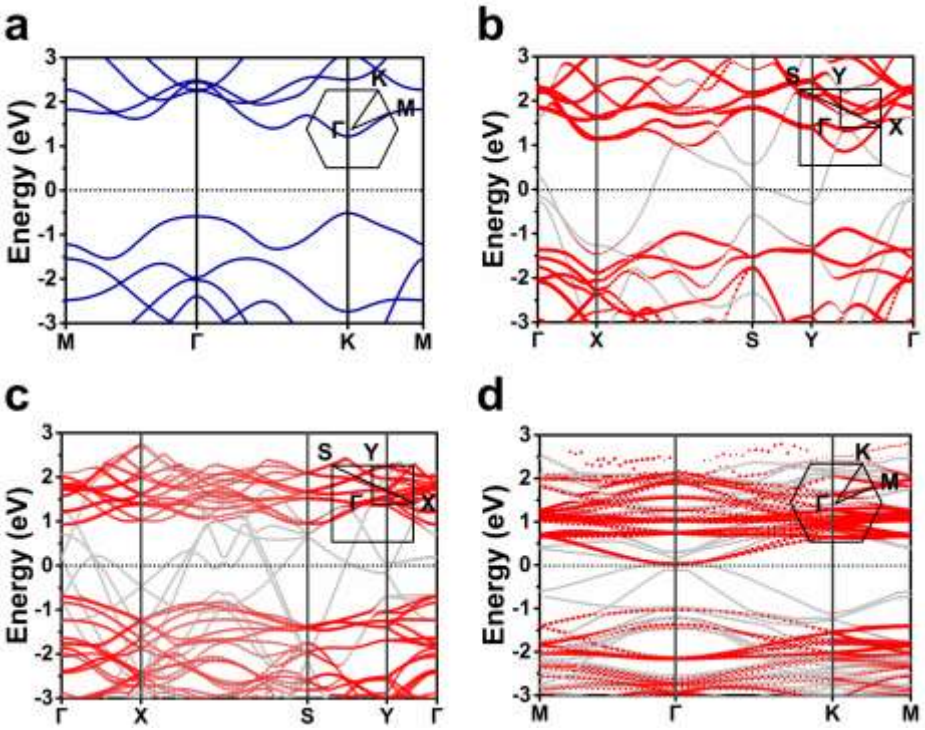

Figure S1. Projected band structures of (a) pristine MoS_2, (b) β_{12}/MoS_2, (c) χ_3/MoS_2 and (f) α'/MoS_2 heterojunctions, with the Fermi levels are set to zero. The band structure calculations are calculated with the GGA + U (U = 2.0 eV) approximation. The red and gray lines in panels b-d indicate the projected energy band of MoS_2 and borophenes, respectively. The Fermi levels (E_f) in panels a–d are represented by the

black dashed lines. The Brillouin zones and high-symmetry paths are denoted in panels a-d.

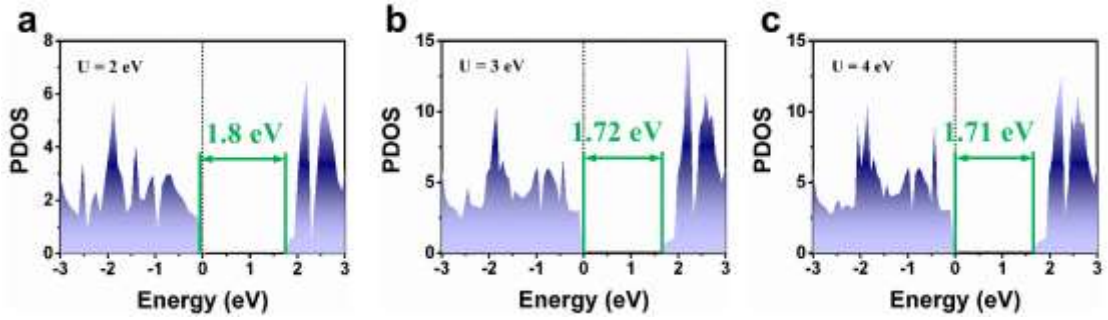

Figure S2 The density of states of pristine monolayer MoS_2 performed with GGA + U approximation with (a) U = 2 eV, (b) U = 3 eV and (c) U = 4 eV, respectively. The band gaps are marked with green arrows.

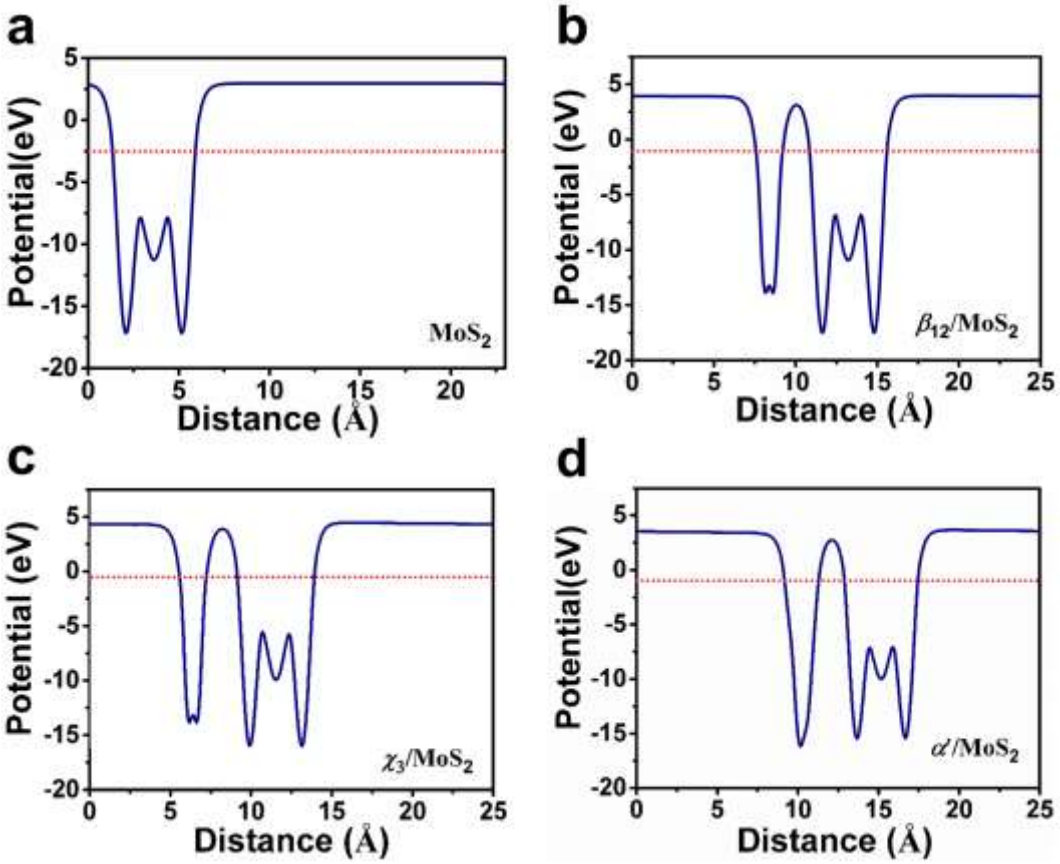

Figure S3. The average electrostatic potential in the perpendicular direction of (a) MoS_2, (b) β_{12}/MoS_2, (c) χ_3/MoS_2 and (d) α'/MoS_2 heterojunctions. The E_f in panels a–d are represented by the red dashed lines. The work functions are 5.47 eV, 5.00 eV, 4.97 eV and 4.97 eV for pristine MoS_2, β_{12}/MoS_2, χ_3/MoS_2 and α'/MoS_2

heterojunctions, respectively.

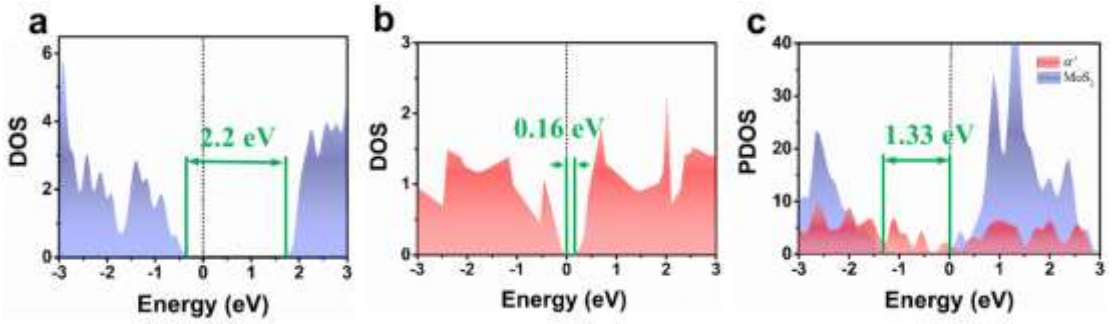

Figure S4 Density of states for (a) MoS_2, (b) α' borophene, and (c) α'/MoS_2, respectively. For clarity, we mark the bandgaps in panels a–c with green arrows. The E_f in panels a–c are represented by the black dashed lines. These calculations are performed with the HSE06 functional.

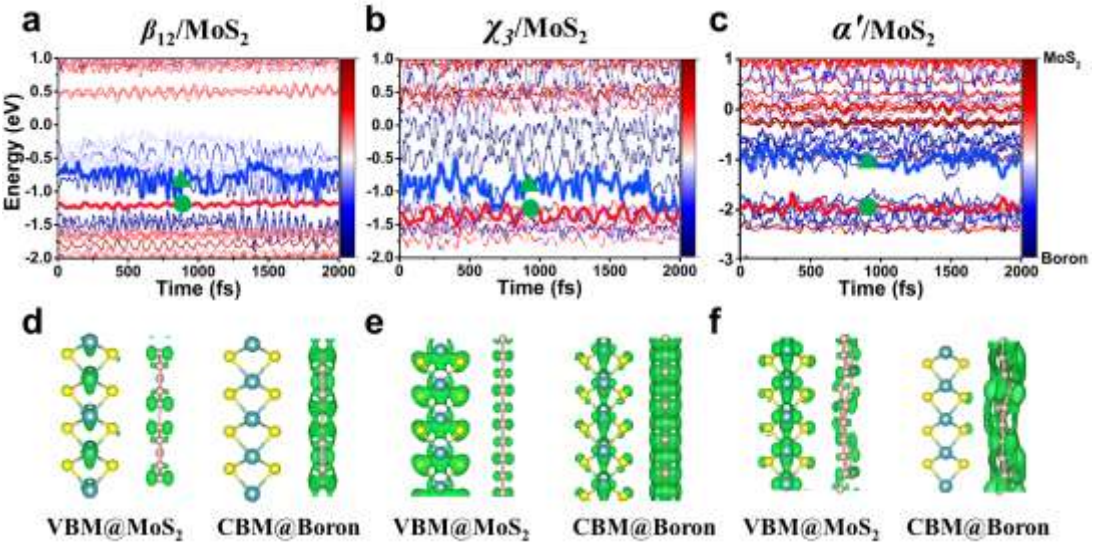

Figure S5. Time-dependent evolution of the energy states of (a) β_{12}/MoS_2, (b) χ_3/MoS_2, and (c) α'/MoS_2 heterojunctions near the conduction band minimum and valence band maximums (VBM). The projected MoS_2 energy states are shown in red, and the projected borophene energy states are shown in blue. The two selected states are VBM@MoS_2 and VBM@borophenes, which are the initial and final states for hole injection, indicated by circles and triangles, respectively. Charge density distributions of the initial and final states for hole injections in the (d) β_{12}/MoS_2, (e) χ_3/MoS_2, and (f) α'/MoS_2 heterojunctions.