Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

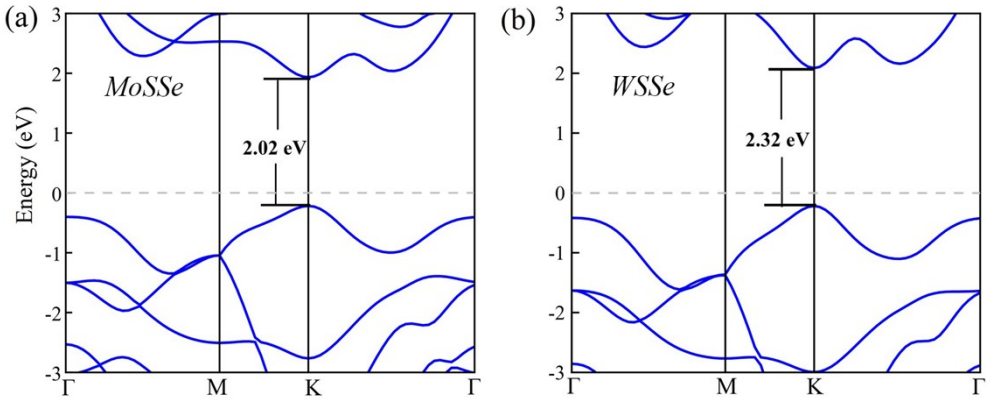

Figure S1. *The HSE06 band structure for (a) Janus MoSSe and (b) WSSe monolayer.*

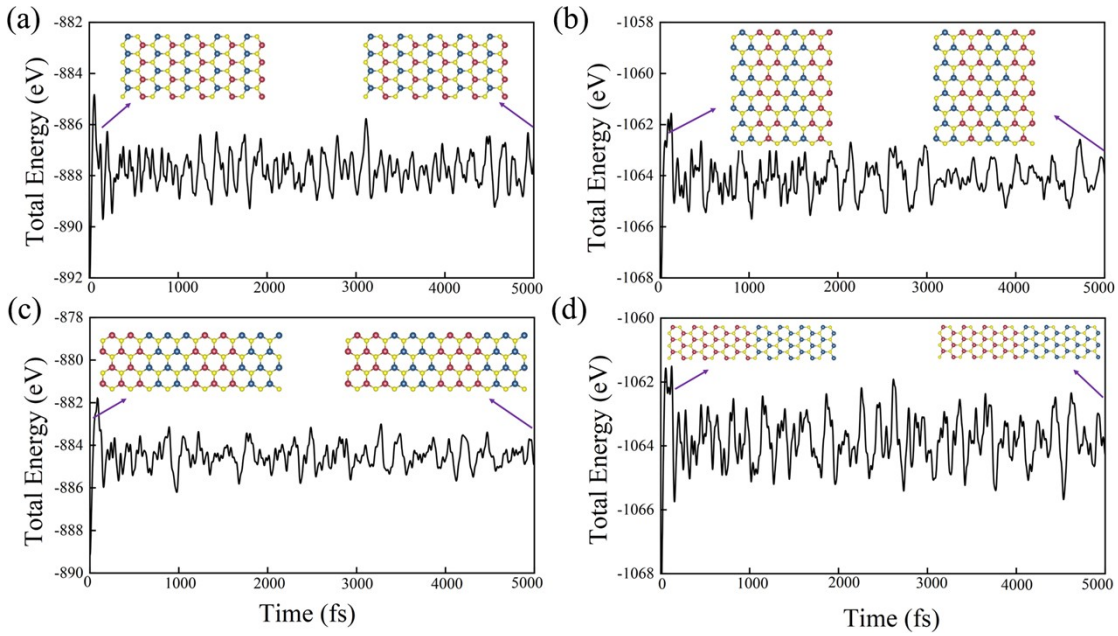

Figure S2. *The AIMD simulation for the Janus superlattices at room temperature. The fluctuation of total energy as a function of relaxation time for (a) $A(Z)_1$-SL, (b)A_3-SL, (c) A_5-SL, and (d) Z_8-SL. The snapshots at the beginning and the end of the structures are also provided.*

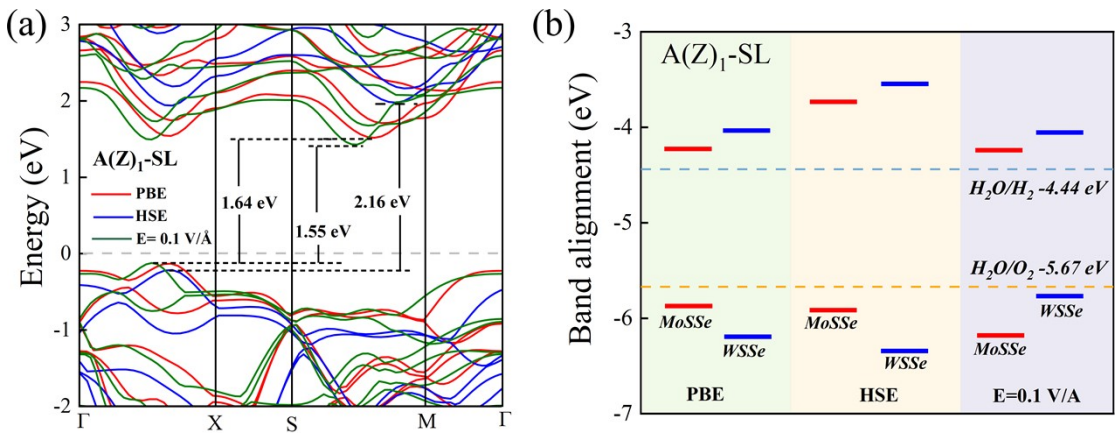

Figure S3. *The band structure and band alignment of $A(Z)_1$-SL in different functional. The band structures (a) calculated by PBE in red, HSE06 in blue, and under an electric field of 0.1V/Å in green, together with the (b) band alignment in different method.*

Table 1. *The HSE06 band gap (E_g) of Janus superlattice in different periodic width N, together with the PBE result for comparison. The symbols I and D in brackets mean indirect and direct, respectively.*

System	***N***	***E_g (eV)***	
		PBE	***HSE***
MoSSe		1.66 (D)	2.02(D)
WSSe		1.79 (D)	2.32(D)
	1	1.64 (I)	2.16(I)
A_N-SL	2	1.71 (D)	2.21(D)
	3	1.63 (D)	2.14(D)
	4	1.66 (D)	2.16(D)
	5	1.67 (D)	2.13(D)
Z_N-SL	2	1.69 (D)	2.19(D)
	3	1.68 (D)	2.18(D)
	4	1.68 (D)	2.15(D)
	5	1.67 (D)	2.12(D)

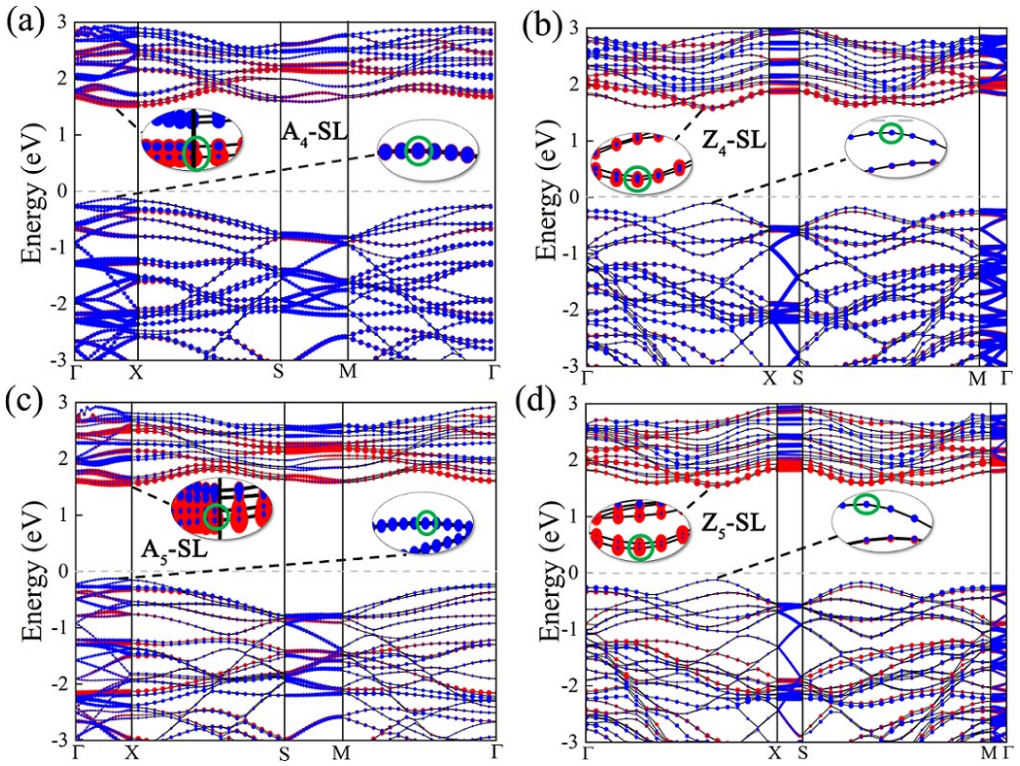

Figure S4. *The band structure for the superlattice (a) A_4-SL, (b) Z_4-SL, (c) A_5-SL, and (d) Z_5-SL. The enlarged part represents the change in the proportion of MoSSe and WSSe of VB and CB, respectively. The red dotted area is contributed by MoSSe, while the blue dotted area is attributed by WSSe. It should be noticed that the circled green part indicates the VBM and CBM points.*

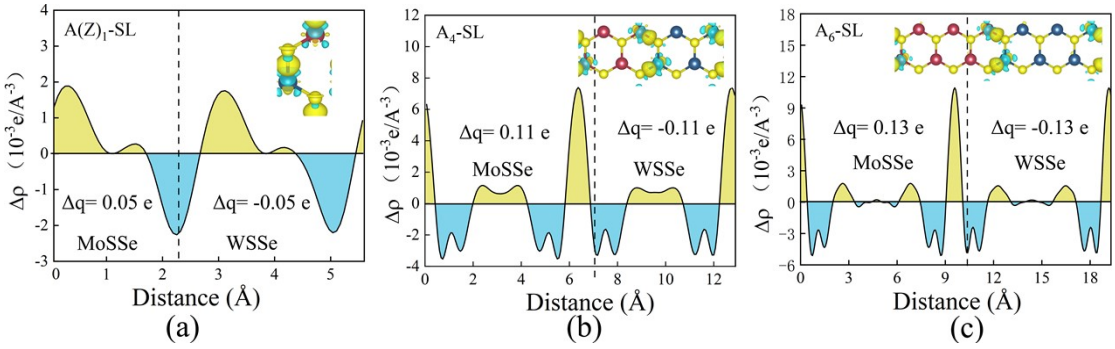

Figure S5. *The projected average electron density difference along the periodic direction for (a) $A(Z)_1$-SL, (b) A_4-SL, and (c) A_6-SL. The blue area represents a depletion of charge, while the yellow area represents the accumulation of charge. Δq represents the amount of charge transferred.*