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Modulating the atomic and electronic structure through alloying and heterostructure of single-layer MoS_2

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Table S1. The *neighboring T-T bonds number*, N_{TT}, correlation functions ($\bar{\Pi}_{2,1}$, $\bar{\Pi}_{2,2}$ and $\bar{\Pi}_{2,3}$) of the SQSs structures, compared with the ideal random solutions.

	$Mo_{0.75}T_{0.25}S_2$		$Mo_{0.5}T_{0.5}S_2$	
	Random	SQS-16	Random	SQS-16
N_{TT}	3	3	12	12
$\bar{\Pi}_{2,1}$	0.25	0.25	0	0
$\bar{\Pi}_{2,2}$	0.25	0.25	0	0
$\bar{\Pi}_{2,3}$	0.25	0.25	0	-0.3333

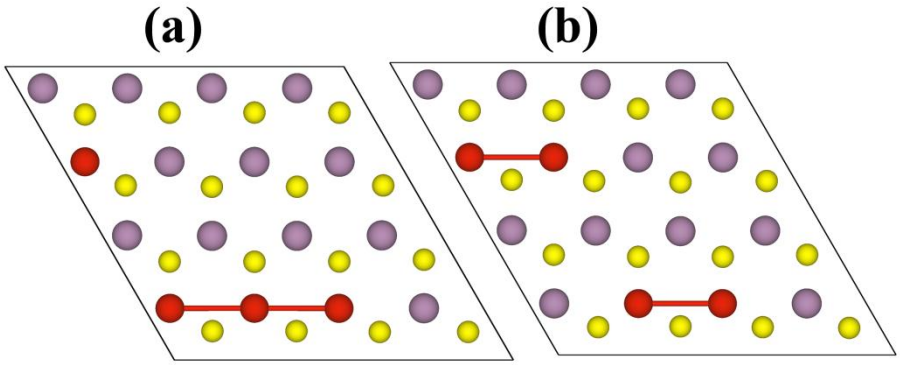

Fig. S1 *Two additional configurations* of $Mo_{0.75}Cr_{0.25}S_2$ considered for checking reliability of SQS: (a) three T atoms connected in a straight line and (b) two parallel pairs of neighboring T atoms.

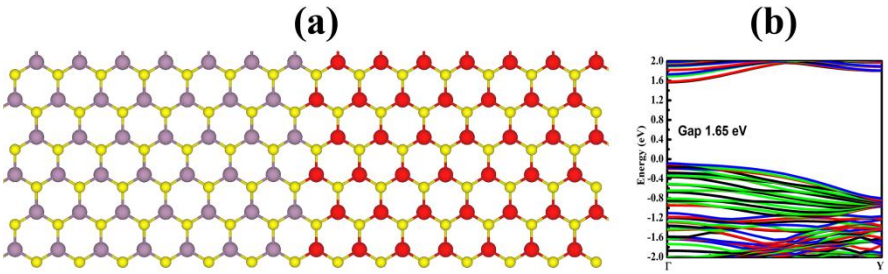

Fig. S2 *The atomic structure (a) and band structure (b) of armchair MoS_2-WS_2 heterostructure with the strip width of 22 Å, as mentioned in the context.*

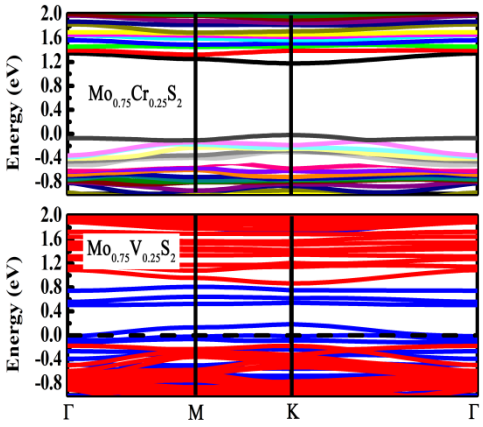

Fig. S3 The calculated band structures of $Mo_{0.75}V_{0.25}S_2$ and $Mo_{0.75}Cr_{0.25}S_2$ with DFT+U (U= 5.95eV, J= 0.95eV). The calculated band gap of $Mo_{0.75}Cr_{0.25}S_2$ is about 1.2 eV.

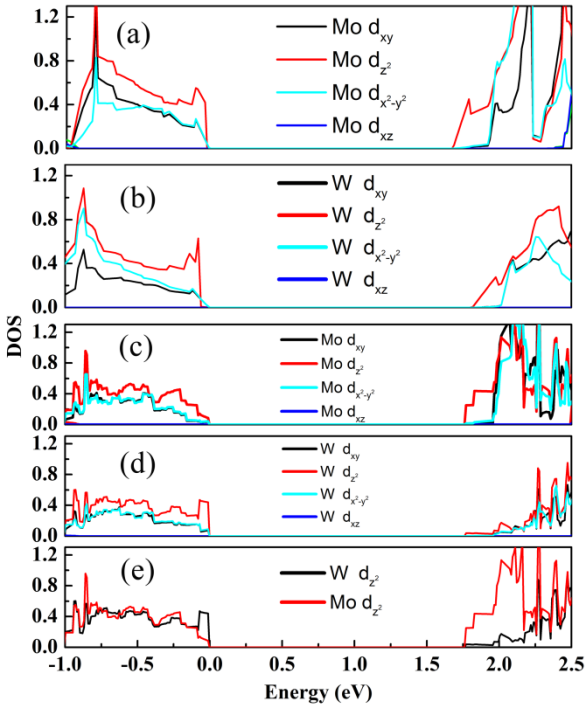

Fig. S4 *Projected density of states(PDOS) of d orbitals for pure MoS_2(a), pure WS_2 (b) and heterostructure of armchair MoS_2-WS_2 (The width of the strip is 12.7 Å, which corresponds to AHS) (c) and (d) show the PDOS of Mo and W atoms of herterstructure. (e) shows the dz^2 of both Mo and W atoms in heterostructure.*