Supporting Information (SI)

Effects of Se substitution and transition metal doping on the electronic and magnetic properties of MoS_xSe_{2-x}/h-BN heterostructure

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Table S1 The value of the magnetic moment $\mu_0(\mu B)$ is the magnetic moment of the free TM atoms, the $\mu_1(\mu B)$ denotes the magnetic moment of the $MoSe_2$/h-BN heterostructure after TM atoms doped and the $\mu_2(\mu B)$ denotes the localized magnetic moment of the TM dopants in the optimized structure. Charge transferfrom the TM atoms to the $MoSe_2$/h-BN heterostructure(**Te**). 4s/3d denote the valence electron configurations for a free-standing TM atom. 4s*/3d*/4p* are the valence electron configurations of the Bader charge analysis relative to the TM atom adsorbed on the surface of $MoSe_2$/h-BN heterostructure.

Atoms	$\mu_0(\mu B)$	$\mu_1(\mu B)$	$\mu_2(\mu B)$	Te	4s/3d	4s*/3d*/4p*
Ni	2.00	0	0	0.31	2/8	0.37/8.62/0.35
V	3.00	5.00	3.04	0.87	2/3	0.35/3.64/0.38
Fe	4.00	2.00	2.28	0.58	2/6	0.35/6.58/0.39
Mn	5.00	3.00	3.14	0.72	2/5	0.25/5.27/0.25
Co	3.00	1.00	1.12	0.40	2/7	0.35/7.56/0.36

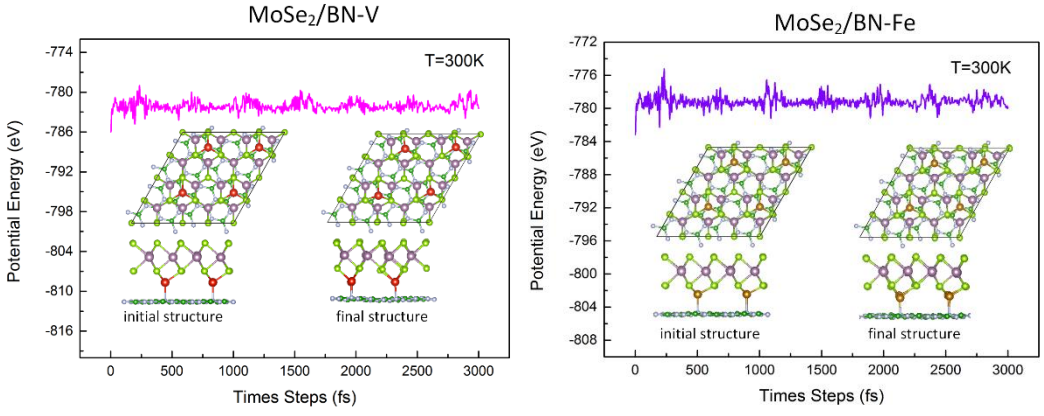

Figure. S1 Molecular Dynamics Simulation of the V- and Fe- doping systems for 300K.

Table S2 The band gap and formation energy of the MoS_2/BN for the 10^{-4} eV/unit cell and 10^{-6} eV/unit cell for 0% and 25% substitutional concentrations with Se atoms.

criteria of energy (eV/unit cell)	substitutional concentration (%)	Band gap (eV)	Energy (eV)
10^{-4}	0	1.019	-200.520
	25	1.148	-198.295
10^{-6}	0	1.028	-200.510
	25	1.150	-198.309

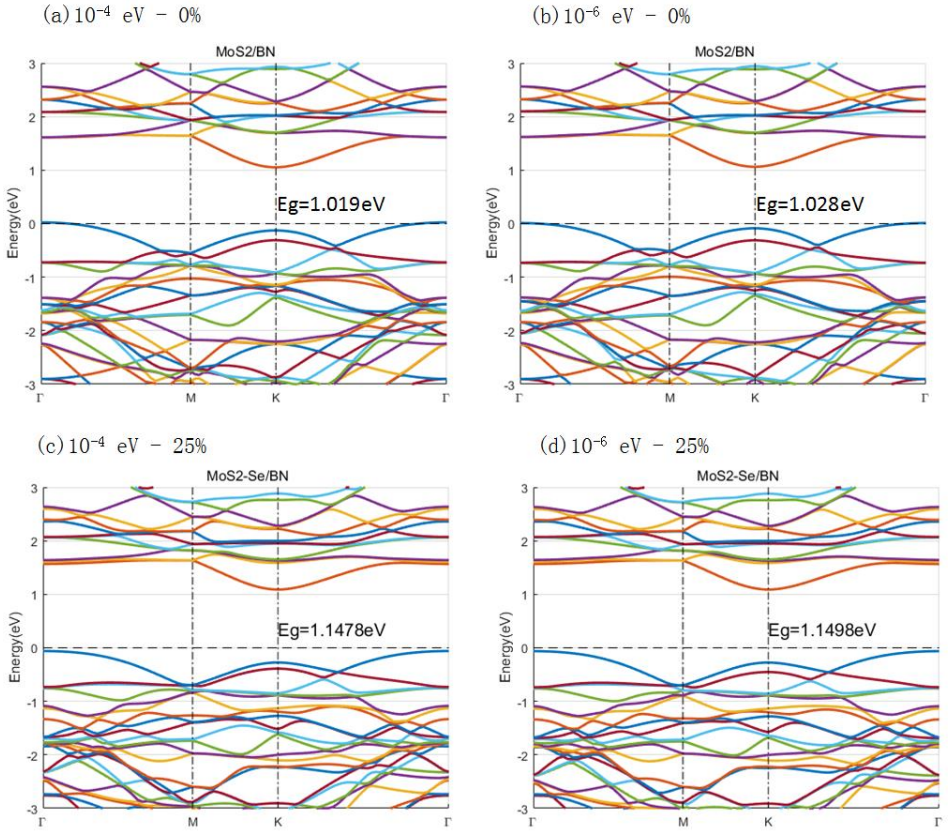

Figure. S2 Band structures of the MoS_2/BN for the 10^{-4} eV/unit cell and 10^{-6} eV/unit cell for 0% and 25% substitutional concentrations with Se atoms.