

Supporting Information

Table. S1 The magnetic moments with corresponding U values (in μ_B).

	Fe _{U=}	Co _{U=}	Ni _{U=}	Ru _{U=}	Rh _U	Pd _{U=}	Os _{U=}	Ir _{U=}	Pt _{U=}
	4eV	4eV	4eV	3eV	=3.4eV	3.9eV	2.7eV	2.8eV	2.9eV
								v	
Mo ₁₅ XS ₃₂	2	3	0	2	1	0	2	1	0
Mo ₁₅ XS ₃₁ -A	0	1	0	0	1	0	0	1	0
Mo ₁₅ XS ₃₁ -B	2	3	0	0	1	2	0	1	0
Mo ₁₅ XS ₃₁ -C	2	1	0	0	1	0	2	1	0
Mo ₁₅ XS ₃₁ -D	2	1	0	0	1	0	0	1	0
Mo ₁₅ XS ₃₁ -E	2	3	0	0	1	0	0	1	0

Table. S2 The energies of non-magnetic states ($E_{\text{non-magnetic}}$ in eV) and magnetic states (E_{magnetic} in eV) of Ni-doped special structure in DFT-PBE and PBE+U.

	DFT-PBE		PBE+U _{U=4eV}	
	$E_{\text{non-magnetic}}$	$E_{\text{magnetic}}(M=4\mu_B)$	$E_{\text{non-magnetic}}$	$E_{\text{magnetic}}(M=4\mu_B)$
Mo ₁₅ NiS ₃₂	-337.325	-337.126	-335.101	-334.951
Mo ₁₅ NiS ₃₁ -B	-330.765	-330.424	-328.466	-328.238
Mo ₁₅ NiS ₃₁ -C	-330.949	-330.594	-328.672	-328.427
Mo ₁₅ NiS ₃₁ -E	-330.633	-330.425	-328.406	-328.244