Electronic Supplementary Material (ESI) for RSC Advances.
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Supplementary Information

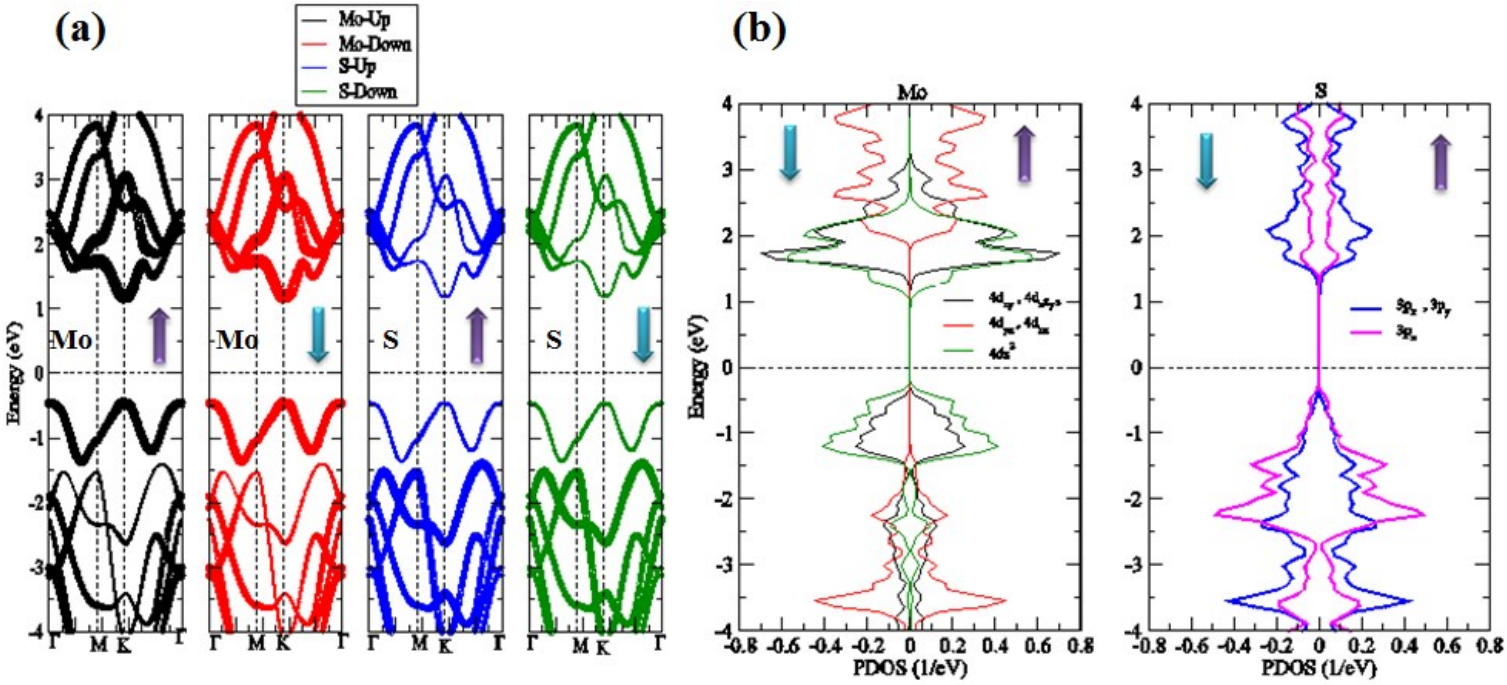

Figure S1: Spin polarized (a) electronic band structure and (b) density of states of the pristine MoS_2. Up and down arrows represents spin up and spin down states, respectively.

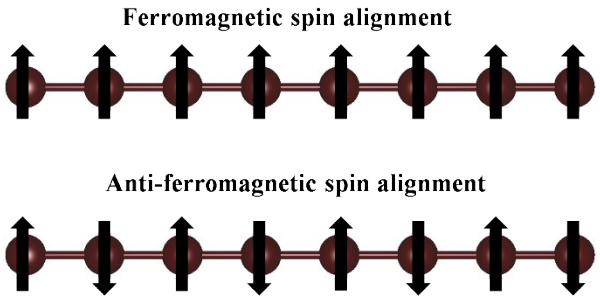

Figure S2: A schematic of spin alignments depicting ferromagnetic (FM) and anti-ferromagnetic (AFM) configurations for monoatomic wires of Fe and Co.

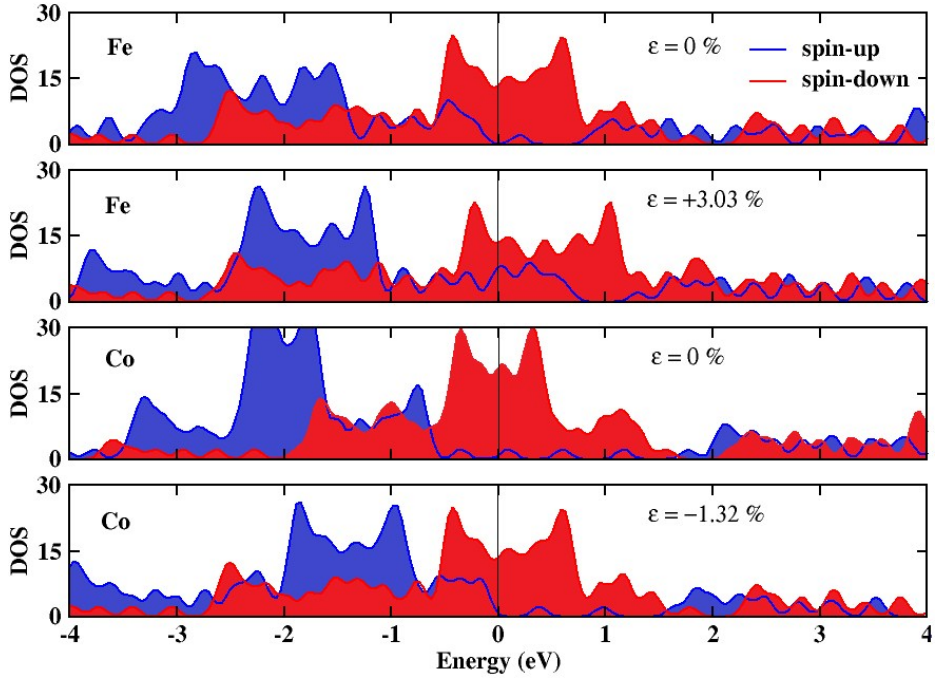

Figure S3: Spin polarized total density of states of the freestanding mono-atomic Fe and Co linear wires. The Fermi level is set at zero and the strain is given by ε. In the functionalized monolayers, there exists strain of +3% and -1.3% in Fe and Co wires, respectively due to lattice mismatch.

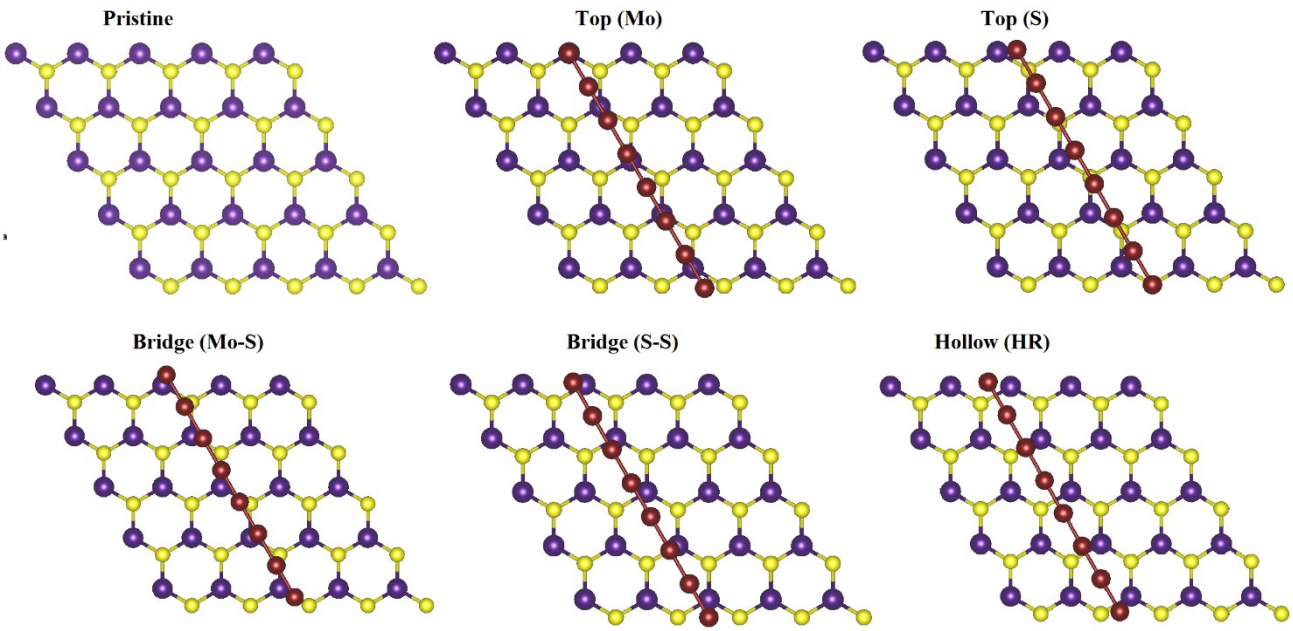

Figure S4: Top view of the functionalized MoS_2 monolayer withdifferent bindingsites. The violet, yellow and brown balls represent Mo, S and atoms of the linear wire, respectively.

Table S1. The binding energy (E_b) and the calculated (average) distance between atomic wire and monolayer ($R_{wire\text{-}MoS2}$) for the functionalized monolayers.

Binding site	**Fe/MoS_2**		**Co/MoS_2**	
	E_b (eV/atom)	$R_{wire\text{-}MoS2}$ (Å)	E_b (eV/atom)	$R_{wire\text{-}MoS2}$ (Å)
Bridge (S-S)	-0.50	1.50	-0.49	1.50
Top (Mo)	-0.40	1.80	-0.43	1.80
Top (S)	-0.37	2.10	-0.41	2.00
Bridge (Mo-S)	-0.38	2.00	-0.41	2.00
Hollow (HR)	-0.32	1.90	-0.35	1.80

Table S2: Bader chargesof the elemental species (Mo, S, Fe and Co) in the pristine and functionalized monolayers. Here subscripts S1 and S2 denote S atoms of the monolayer which are distant and near to atomic wires in the functionalized system. (Bader charges per atom can be calculated by dividing the presented values for Mo, S1, S2 by 25 and Fe/Co by 8.)

Monolayer	**Bader Charges (e)**			
	q_{Mo}	q_{S1}	q_{S2}	$q_{Fe/Co}$
MoS_2	-1.04	+0.52	+0.52	-
Fe@MoS_2	-0.28	+0.37	+1.85	-1.94
Co@MoS_2	-0.28	+0.37	+1.85	-1.95

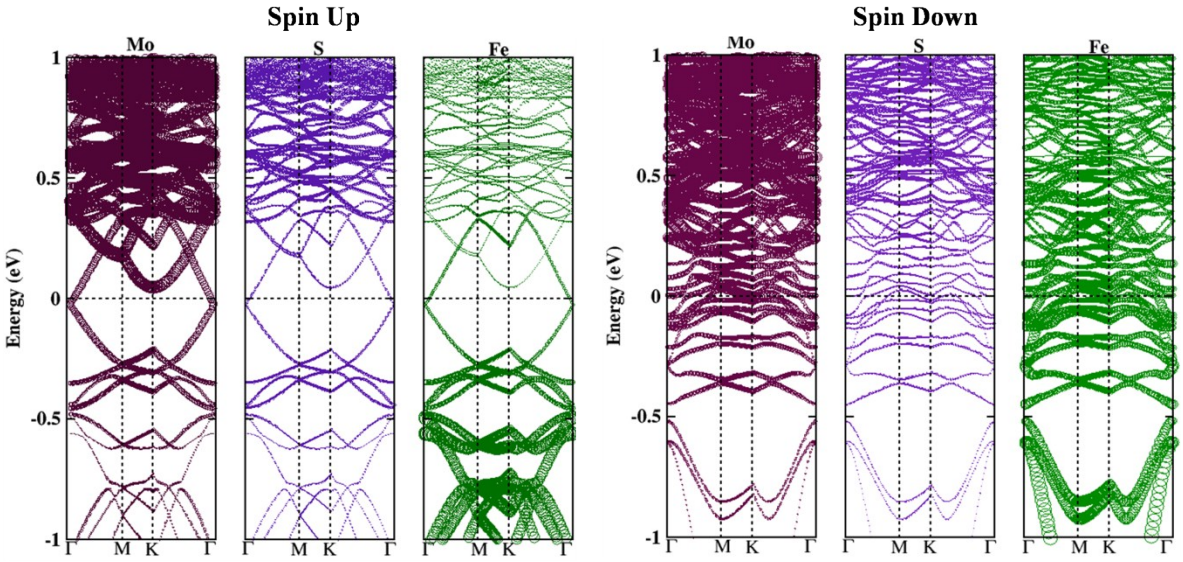

Figure S5: Projected spin-polarized band structures of the Fe functionalized monolayer. The width of the bands depicts spectral weight of the points.Fermi Energy is set at 0 eV.

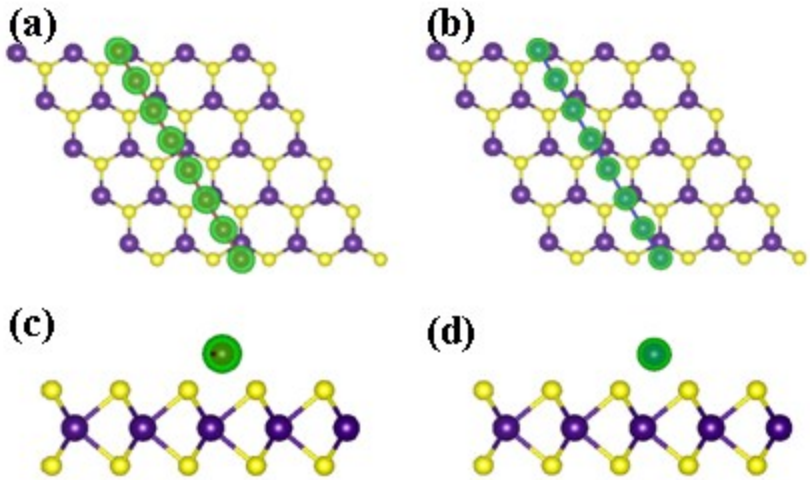

Figure S6. The spin-up density plots for Fe/MoS_2 (a and c) and Co/MoS_2 (b and d). Isosurface values are set at 0.05 e/(Å)^3.

Table S3: Calculated adsorption energies (E_{ads}) of the TM atoms adsorbed on the MoS_2 monolayer at the most stable adsorption sites [a], the total magnetic moments (μ_{total}) of the system, the magnetic moments of the adatom (μ_{adatom}).

Add Atom	**Adsorption Site**	**Adsorption Energy (eV)**	**Toal Magnetic Moment**	**Magnetic moment per add atom**
Fe	Top of Mo	1.57, 2.30 [a]	1.89, 1.99 [a]	2.44, 2.11 [a]
Co	Top of Mo	2.76, 2.70 [a]	0.88 , 0.99 [a]	0.77, 0.96 [a]

[a] Wang et al. Physica E 63 (2014) 276–282