Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information

First-principles study of phase transition and the structural, energetic and electronic properties of pristine and transition metal (Fe/Co/Ti)-doped layered MoS_2 as anode materials for sodium-ion batteries

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Table S1: Pristine and TM-doped MoS_2 optimized lattice parameters (a, b, c, α, β, γ), and average atom distance of Mo-S (d_{Mo-S}) and M-S (d_{M-S})

	Phase	a(Å)	b(Å)	c(Å)	α(°)	β(°)	γ(°)	d_{M-S} (Å)	d_{Mo-S} (Å)
Pristine	1T	6.51	6.51	12.09	90	90	120	-	2.44
	2H	6.40	6.40	12.42	90	90	120	-	2.42
Fe	1T	6.50	6.50	11.85	90	90	120	2.32	2.43
	2H	6.39	6.39	12.34	90	90	120	2.34	2.42
Co	1T	6.51	6.51	11.79	90	90	120	2.31	2.43
	2H	6.41	6.41	12.33	90	90	120	2.34	2.42
Ti	1T	6.50	6.50	11.97	90	90	120	2.42	2.43
	2H	6.45	6.45	12.24	90	90	120	2.41	2.42

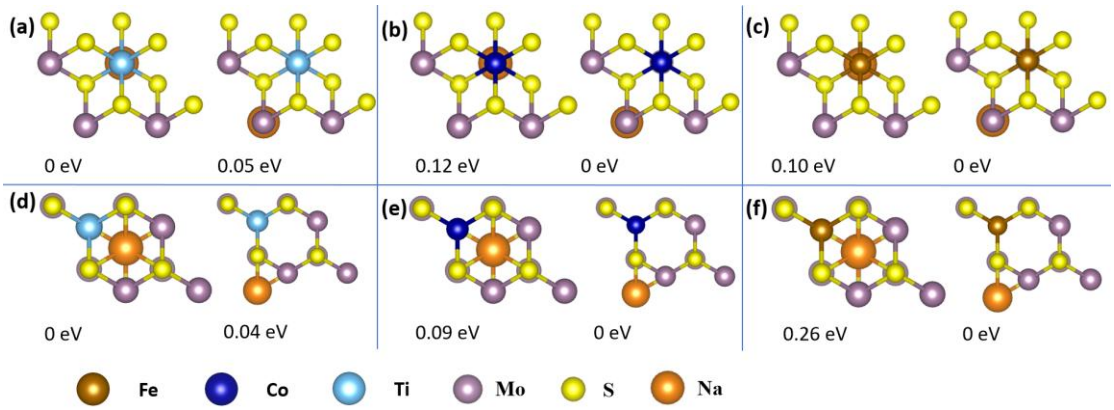

Fig. S1. The system relative energy of single Na atom intercalation in (a) Ti-doped (b) Co-doped and (c) Fe-doped 1T phase MoS_2, (d) Ti-doped (e) Co-doped and (f) Fe-doped 2H phase MoS_2. The configuration on the left is close to M, and the configuration on the right is far from M. The lower energy configuration is set to 0 eV.

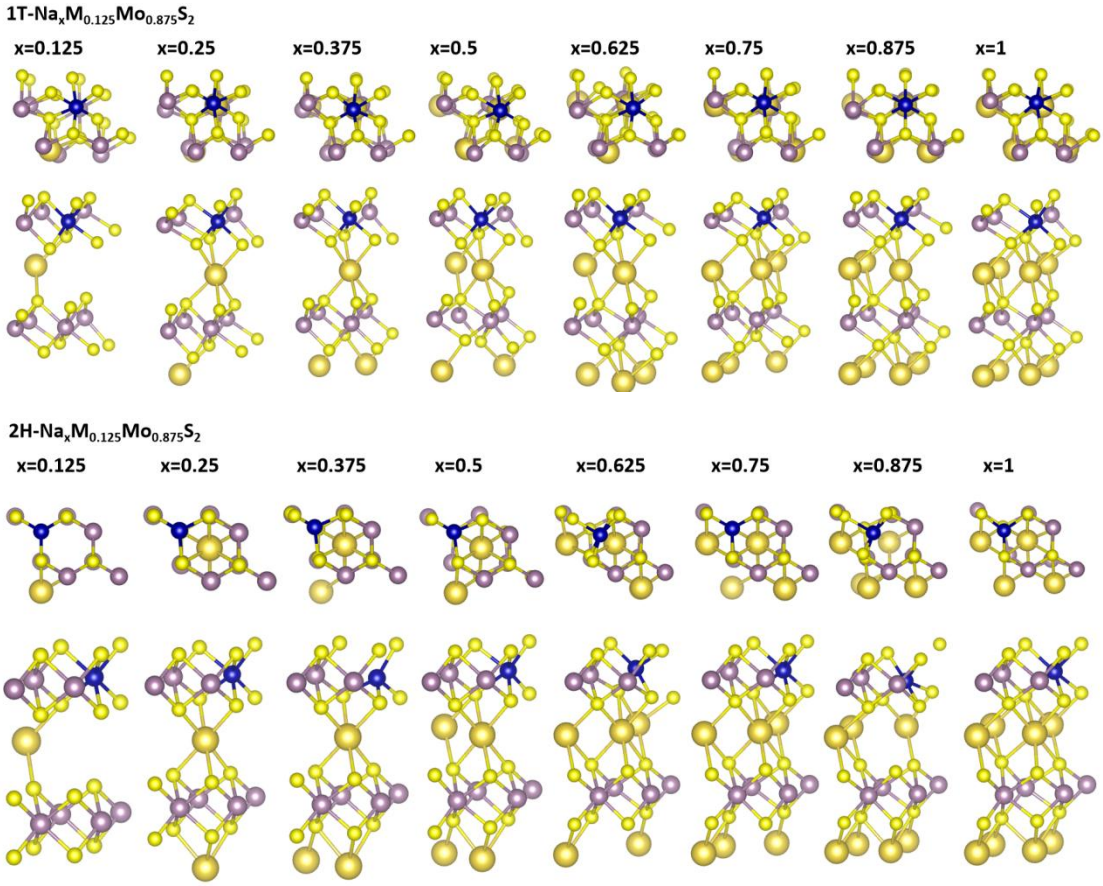

Fig. S2. TM-doped MoS_2 with Na intercalation. Mo is in purple, S is in light yellow, M (Fe/Co/Ti) is in blue, and Na is in dark yellow.

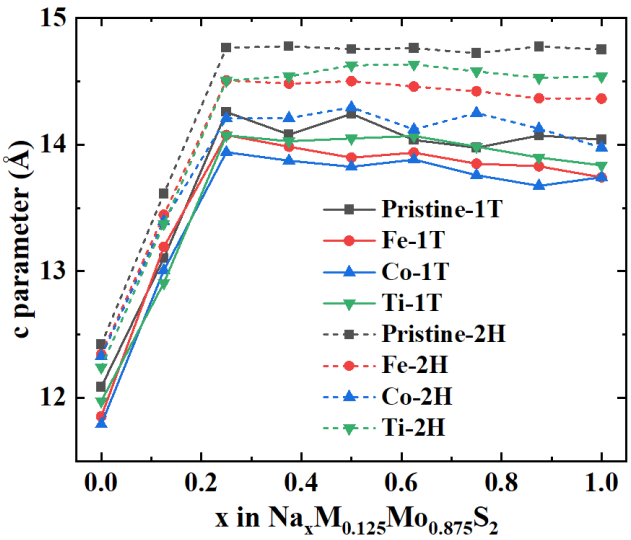

Fig. S3. The lattice parameters c with different Na concentration intercalation for 1T and 2H $M_{0.125}Mo_{0.875}S_2$.

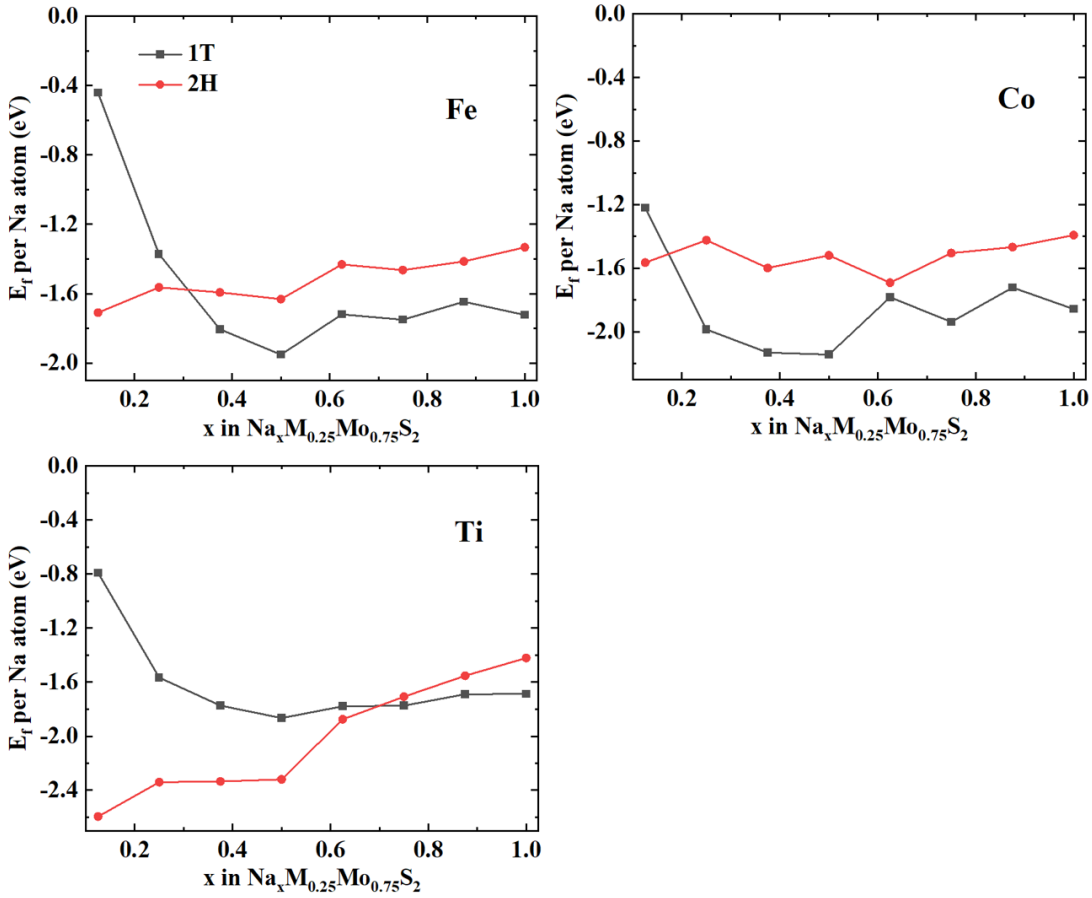

Fig. S4. Formation energy per Na atom for 1T and 2H $Na_xFe_{0.25}Mo_{0.75}S_2$, $Na_xCo_{0.25}Mo_{0.75}S_2$, and $Na_xTi_{0.25}Mo_{0.75}S_2$.