Supporting Information

Defect Induced Performance Enhancement of Monolayer MoS_2 for Li- and Na-Ion Batteries

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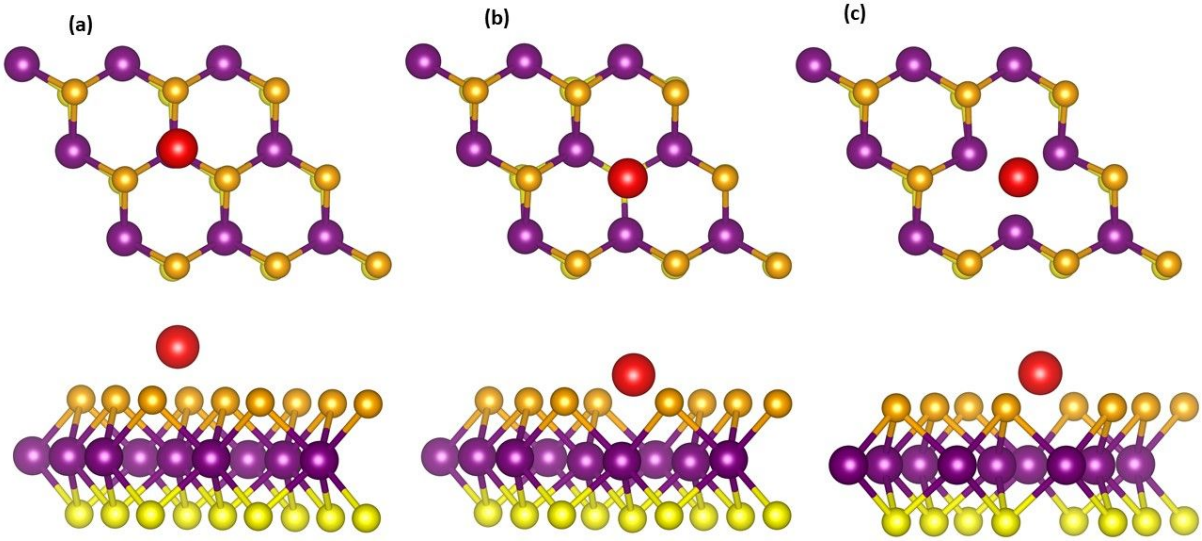
Figure S1: Optimized geometry of Li adsorbed at defective sites of monolayer MoS_2 with various types of defects. (a) Pristine MoS_2, (b) Mono sulphur vacancy, (c) di sulphur vacancy, (d) Mo vacancy, (e) MoS_3 vacancy, (f) MoS_6 vacancy (g) Mo_{S2} vacancy and (h) $S2_{Mo}$ vacancy. The purple, yellow and red balls represent Molybdenum, Sulphur and Lithium atoms respectively. The top layer of S atoms is in golden yellow colour and bottom layer are in light yellow colour.



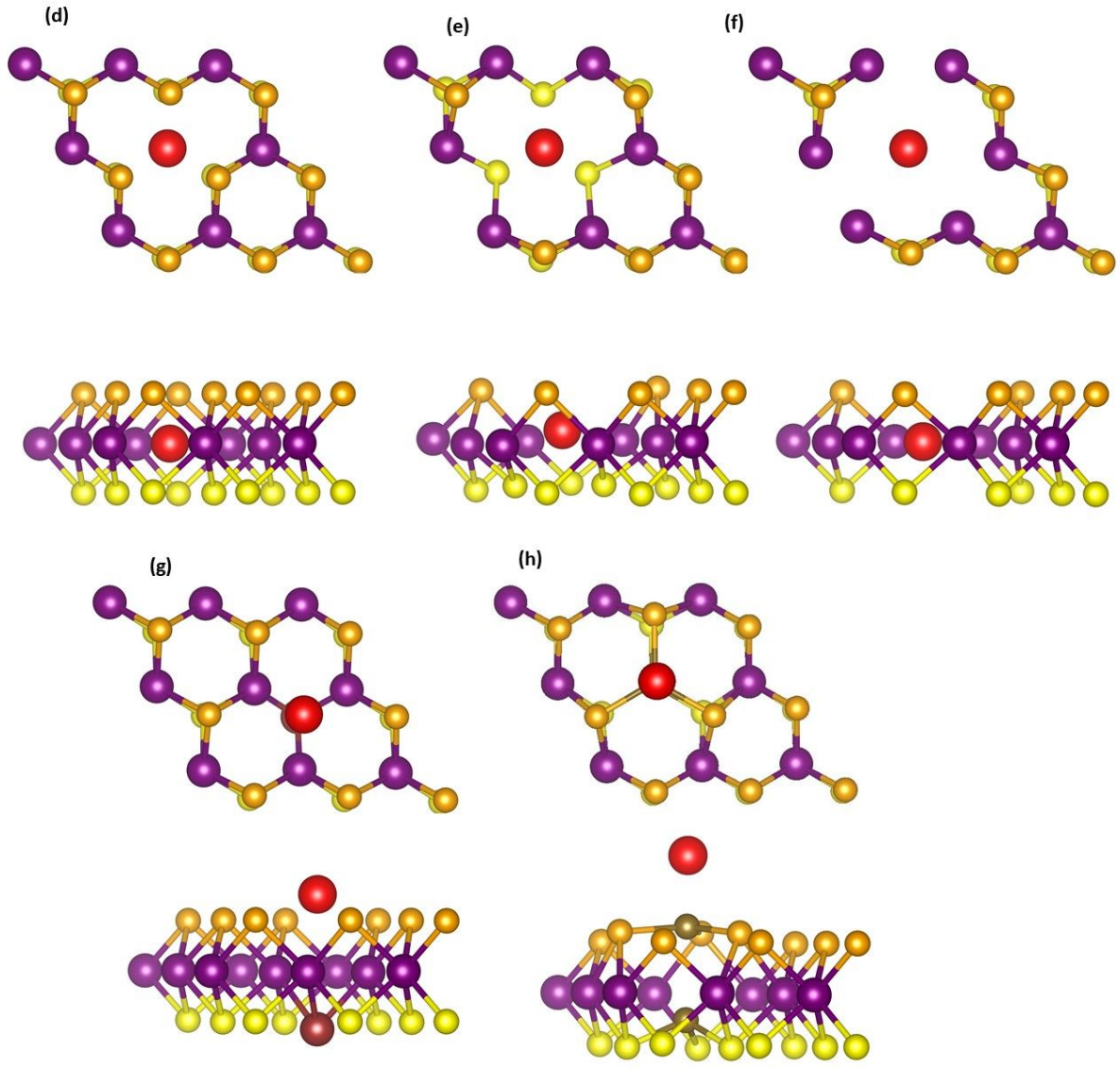
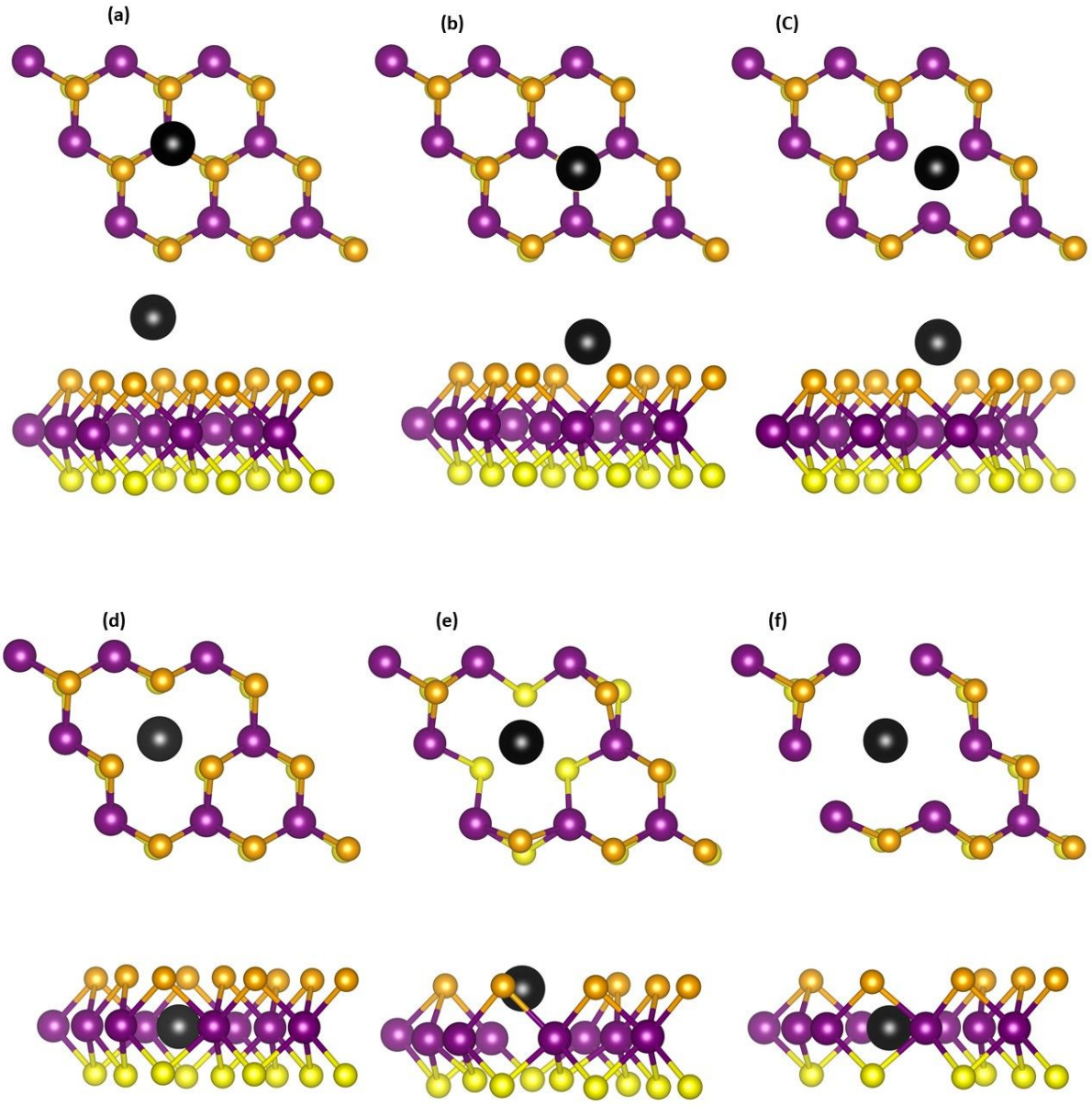


Figure S2: Optimized geometry of Na adsorbed at defective sites of monolayer MoS_2 with various types of defects (a) Pristine MoS_2, (b) Mono sulphur vacancy, (c) di sulphur vacancy, (d) Mo vacancy, (e) MoS_3 vacancy, (f) MoS_6 vacancy, (g) Mo_{S2} vacancy and (h) $S2_{Mo}$ vacancy. The purple, yellow and red balls represent Molybdenum, Sulphur and sodium atoms respectively. The top layer of S atoms is in golden yellow colour and bottom layer are in light yellow colour.


(a)
(b)
(C)
(d)
(e)
(f)

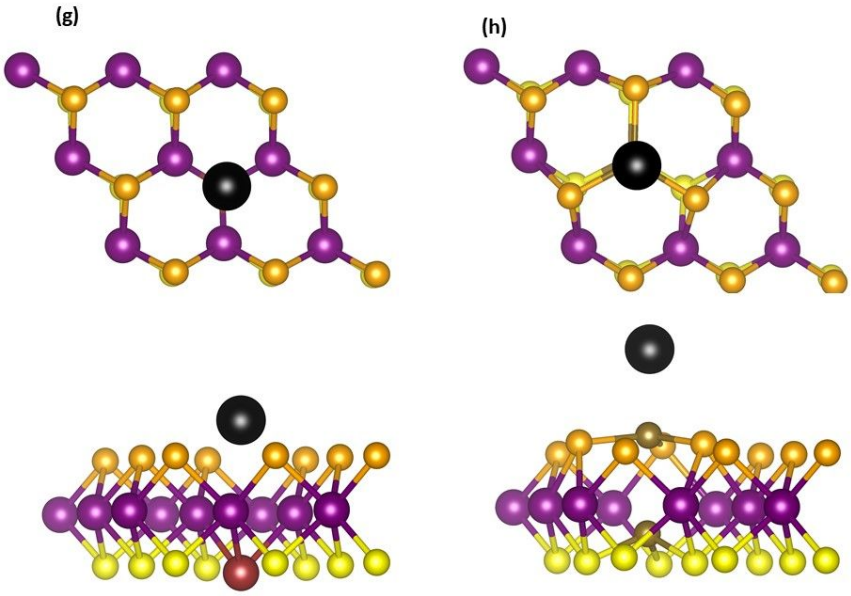
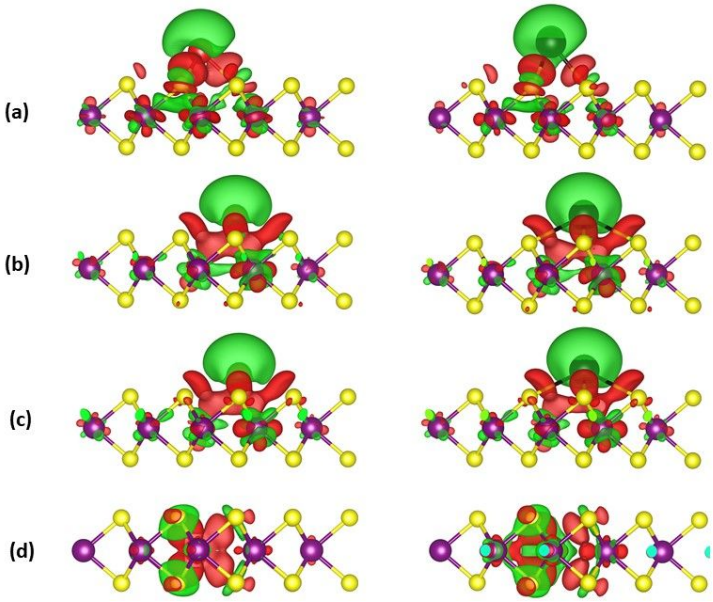


Figure S3: Charge density difference isosurface plots for Li (left) and Na (right) adsorption on monolayer MoS_2 with various types of defects. (a) Pristine MoS_2, (b) Mono sulphur vacancy, (c) di sulphur vacancy, (d) Mo vacancy, (e) MoS_3 vacancy, (f) MoS_6 vacancy (g) Mo_{S2} vacancy and (h) $S2_{Mo}$ vacancy. yellow S, purple Mo, red Li and black Na. Red and green regions represent electron accumulation and depletion, respectively.



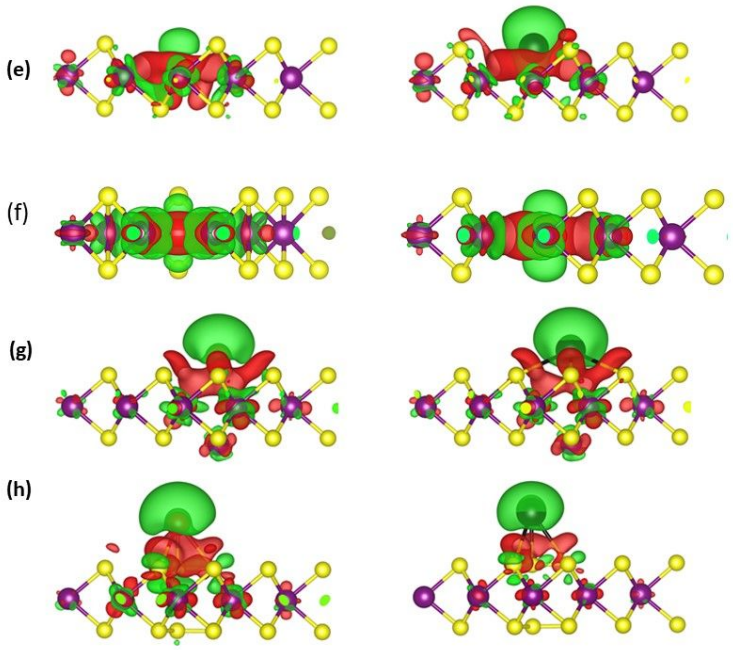
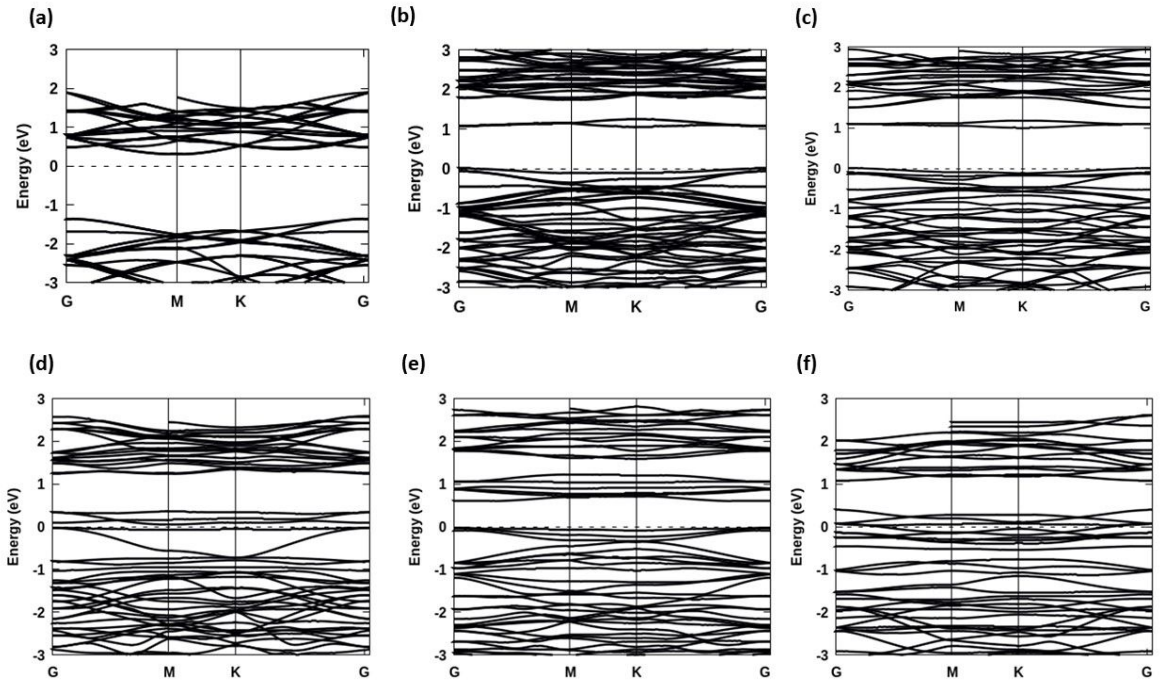


Figure S4: Band structure diagrams of various defects in monolayer MoS_2. (a) Pristine MoS_2, (b) Mono sulphur vacancy, (c) di sulphur vacancy, (d) Mo vacancy, (e) MoS_3 vacancy, (f) MoS_6 vacancy (g) $S2_{Mo}$ vacancy and (h) Mo_{S2} vacancy.



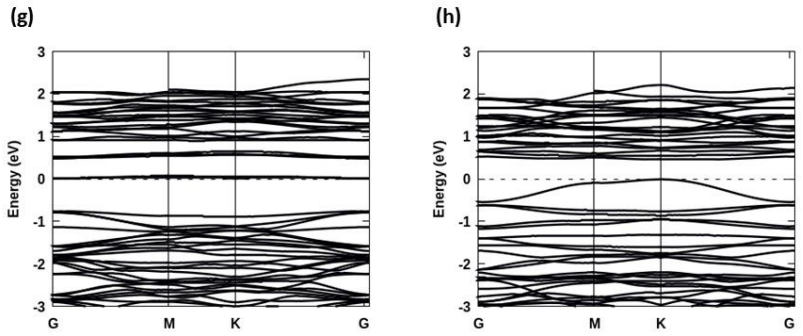


Table S1: The calculated vacancy formation energy (eV), Optimized lattice constant (Å), Energy gap (eV) and magnetic moment (μ_B) of various types of defective and pristine MoS_2.

Vacancy	Vacancy formation energy (eV)	Optimized lattice constant in a_0 (Å)	Energy gap E_g (eV)	Magnetic moment (μ_B/cell)
Pristine MoS_2	---	3.19	1.67	0.00
V_{1S}	1.95	3.18	1.06	0.02
V_{2S}	3.78	3.15	1.02	0.07
V_{Mo}	5.73	3.17	0.09	0.22
V_{MoS3}	7.9	3.19	0.64	0.04
V_{MoS6}	13.89	3.06	0.03	2.25
Mo_{S2}	6.89	3.16	0.01	2.00
$S2_{Mo}$	9.33	3.26	0.48	0.00

Table S2: Effect of magnetism on adsorption energy of Li/Na when adsorption takes place with various types of defective and pristine MoS_2.

Defects	E_{ad} (Li) in eV		E_{ad} (Na) in eV	
	Without magnetism	With magnetism	Without magnetism	With magnetism
Pristine MoS_2	-2.08	-2.08	-1.28	-1.28

V_{1S}	-2.53	-2.57	-1.96	-1.99
V_{2S}	-2.42	-2.44	-1.87	-1.89
V_{Mo}	-3.90	-3.92	-1.80	-1.81
V_{MoS3}	-2.82	-2.83	-2.10	-2.09
V_{MoS6}	-3.37	-3.37	-2.30	-2.28
Mo_{S2}	-2.78	-2.58	-2.19	-1.99
$S2_{Mo}$	-3.08	-2.28	-1.39	-1.61