Supporting Information for

Hydrogen atom induced magnetic behaviors in two-dimensional materials: Insight on origination in the model of α-MoO_3

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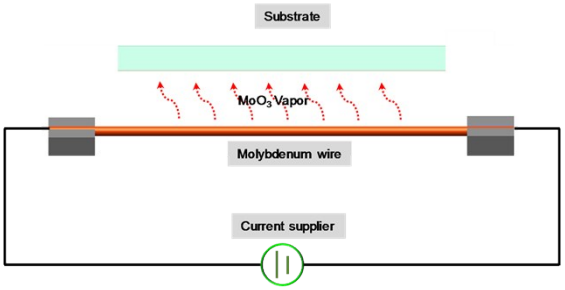

Fig. S1. Schematic of the home-made resistive heating setup to synthesize α-MoO_3 nanosheets.

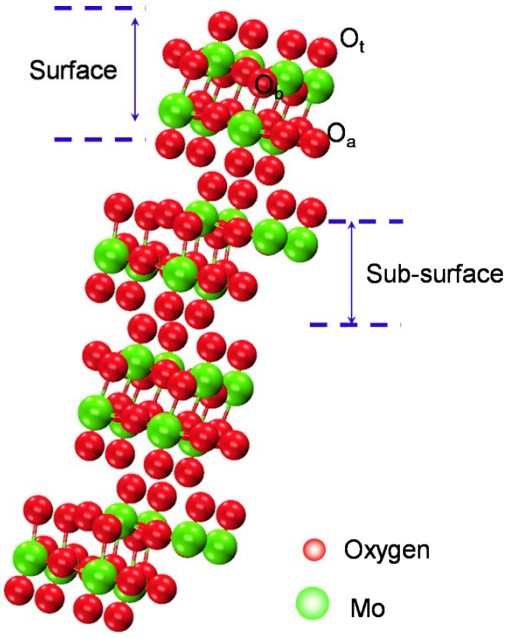

Fig. S2. Schematic view of the calculated prototypical α-MoO_3 structure.

Table S1 The relative energies corresponding to all possible configurations for hydrogen doped α-MoO_3.

Add one extra H	Type	Total Energy (eV)	Δ E (kcal/mol)
surface	terminal	-1056.3644	3.83735
	bridge1	-1056.4809	1.15074
	bridge2	-1056.1780	8.13592
sub-surface	terminal	-1056.5308	0.00000
	bridge1	-1056.5231	0.17757
	bridge2	-1056.1684	8.35731

Table S2 The relative energies corresponding to all possible configurations for α-MoO_3 with one oxygen vacancy.

Remove one O	Type	Total Energy (eV)	Δ E (kcal/mol)
surface	terminal	-1045.1462	0.00000
	bridge1	-1044.9902	3.59752
	bridge2	-1043.4622	38.83472
sub-surface	terminal	-1045.1427	0.08071
	bridge1	-1044.9543	4.42541
	bridge2	-1044.9717	4.02414

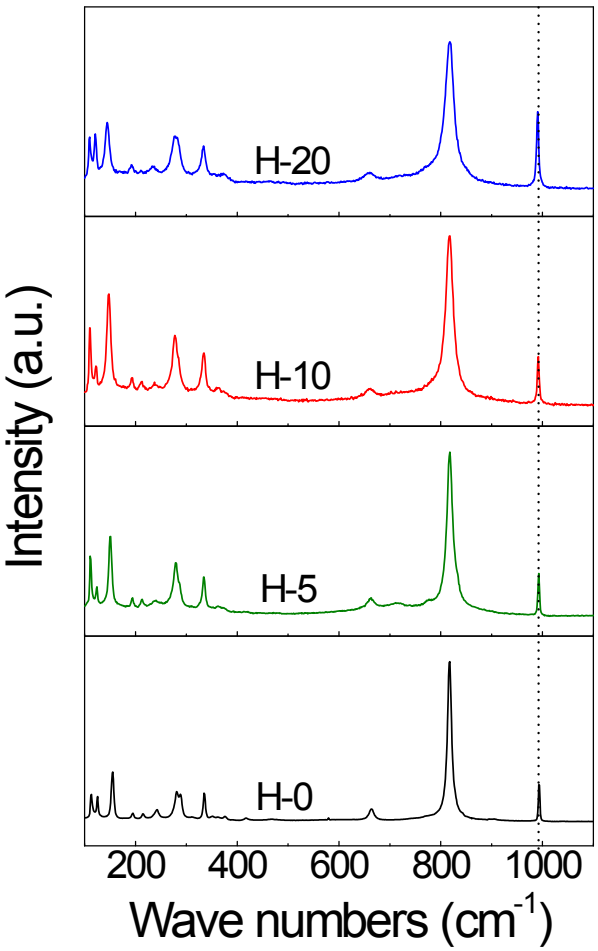

Fig. S3. (a) Raman spectrum of pristine and hydrogenated α-MoO_3.

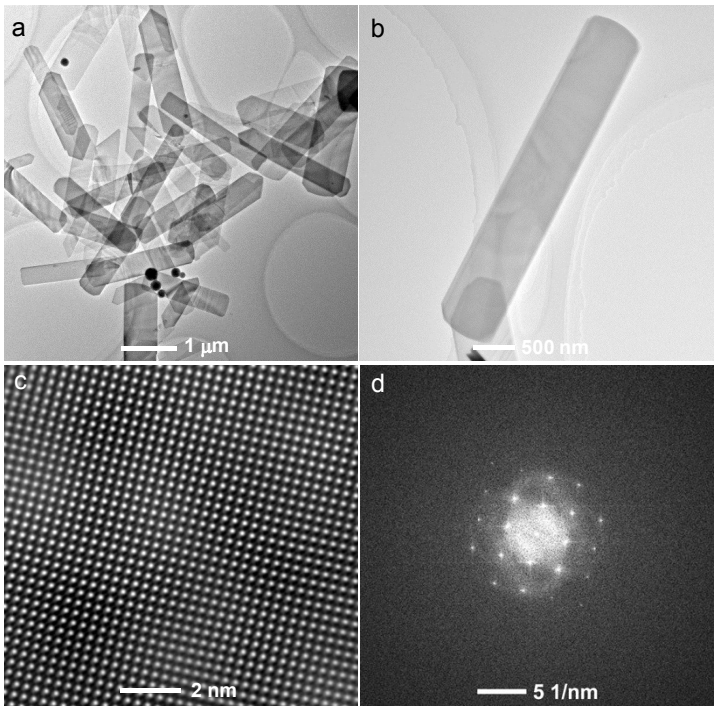

Fig. S4. (a) Representative TEM image (b) High magnification TEM image, (c) HRTEM image, (d) Corresponding FFT pattern of the pristine α-MoO_3 nanosheets.

Fig. S4a shows a representative TEM image of pristine α-MoO_3 nanosheets. We find that the α-MoO_3 nanosheets has a high dispersion, uniform size and smooth surface. The high magnification TEM image in Fig. S4b shows that the length and width of the nanosheets are about 10 μm and 650 nm, respectively. The thickness of α-MoO_3 NB is about 6.8 nm with a 4-layered structure which has been studied in our previous study[12]. The high-resolution TEM image and corresponding FFT data both reveal the single crystallinity nature of the pristine α-MoO_3 nanosheets (Fig. 1e-g), without any impurity, stacking faults or amorphous region.

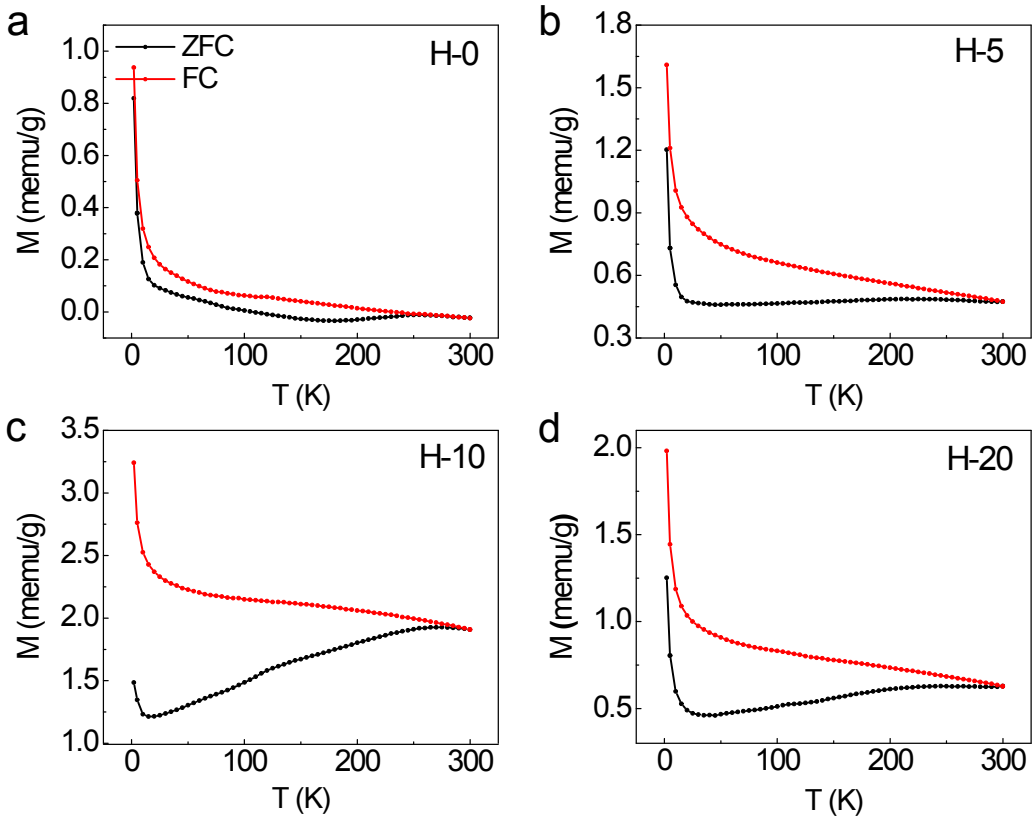

Fig. S5. Temperature-dependent ZFC and FC magnetization curves for pristine and hydrogenated α-MoO_3 samples in a field of 500 Oe.

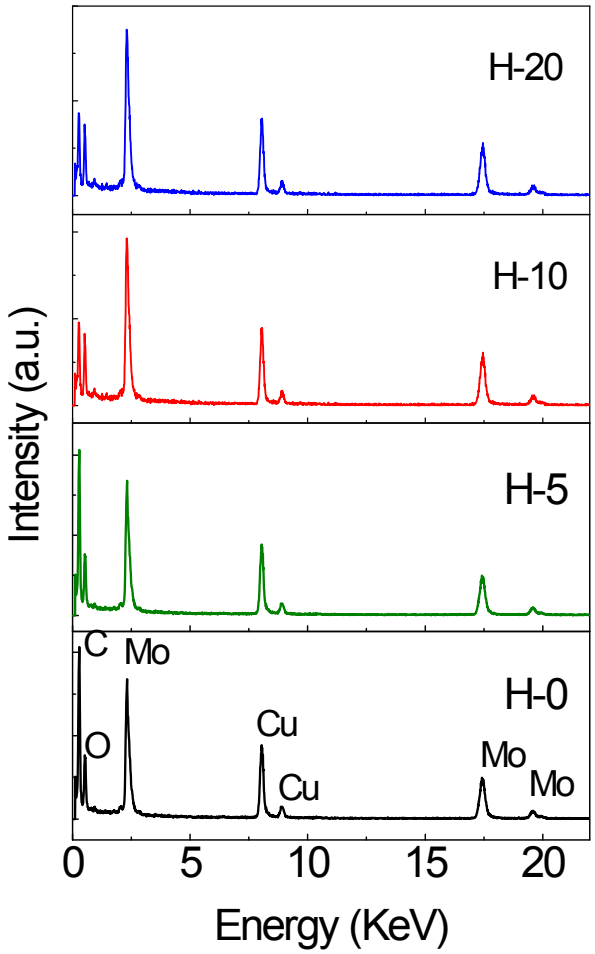

Fig. S6. (a) EDX spectra of pristine and hydrogenated α-MoO_3. The spectra indicate that the samples compose of Mo and O, where the content of Cu and C come from the TEM grid.

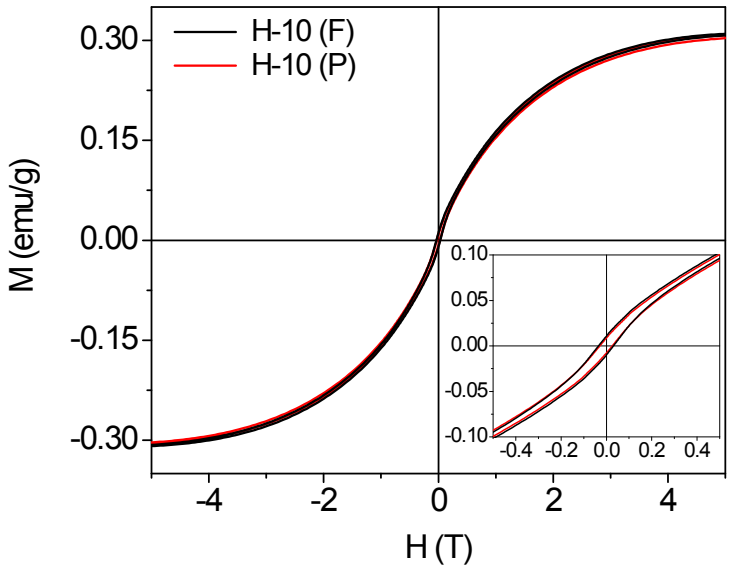

Fig. S7. Hysteresis loops of fresh H-10 (black line) and preserved for 30 days (red line), and no obvious difference was observed. The stability of ferromagnetism is confirmed by the hysteresis loops, where there is no obvious difference between the samples.

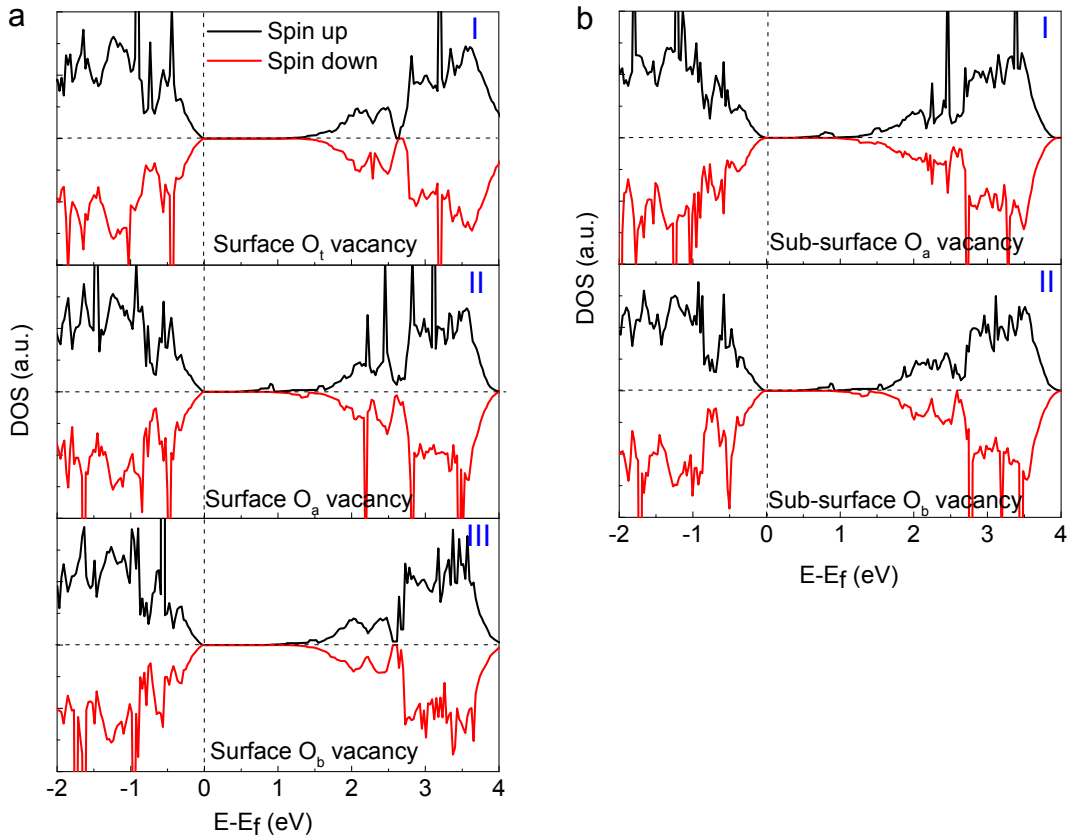

Fig. S8 Calculated density of state (DOS) structure for MoO_3 with one oxygen vacancy.

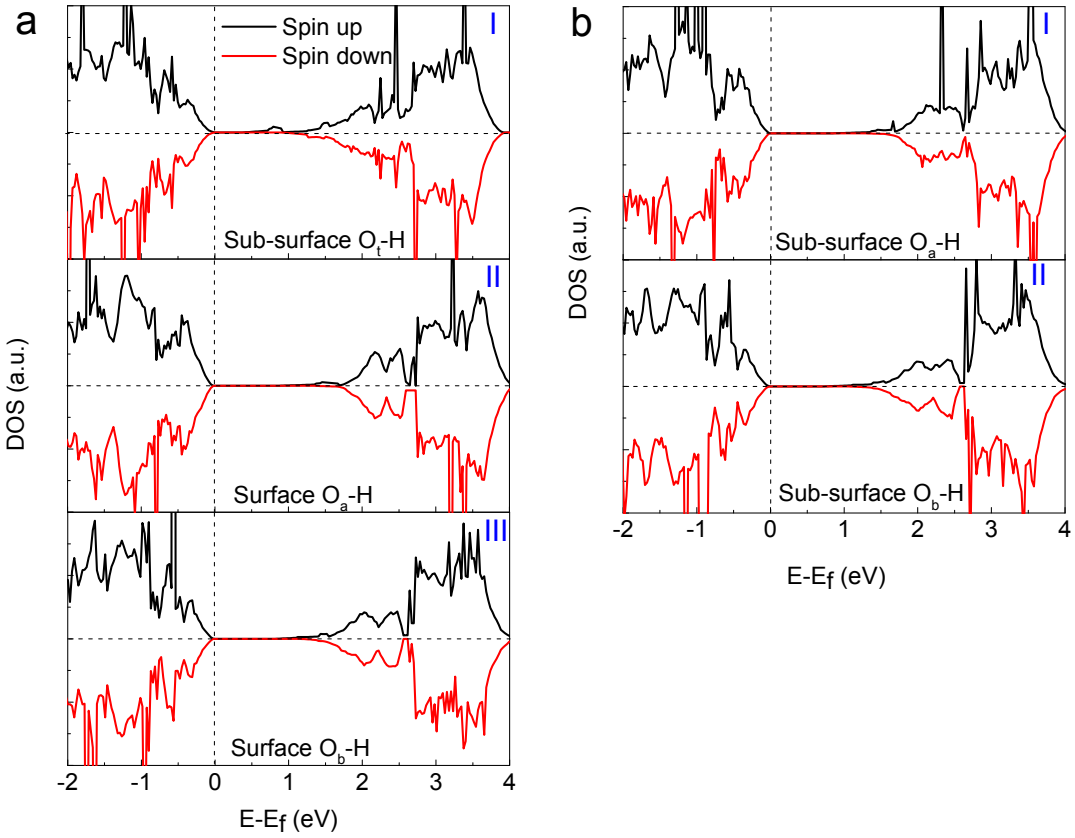

Fig. S9 Calculated density of state (DOS) structure for hydrogen doped MoO_3.