Supplementary data

Modulating Surficial Oxygen Vacancy of VO2 Nanostructure to

Boost Its Electromagnetic Absorption Performance

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1. Experimental section

*Preparation of MoO*₃-*B*_{0.5}: Prepare commercial MoO₃ (1 g) and NaBH₄ (0.5 g) to a mortar, and then grinding the solid mixture using pestle for 20 min until it turns black. Instantaneously, transfer the solids mixture from the mortar into a beaker of cold water. Then stirring for 1 h until no bubbles appear in the solution, indicating that excess NaBH₄ has been removed. The final precipitations are collected by vacuum filtration and wash with methanol and distilled water twice times, and then dry in a vacuum at 60°C for 12 h.

2. Supported table

Table S1. The area of the corresponding individual component is fitted by the peak for VO₂ and VO₂-B_x (x = 0.05, 0.3, 1.0).

	V4+ 2p3/2	V5+ 2p3/2	V4+ 2p1/2	V5+ 2p1/2	O1s	ОН
VO ₂	11900.622	13599.736	6637.54	6095.68	23375.79	7553.521
VO ₂ -B _{0.05}	14186.112	10787.608	5093.46	5164.53	15501.81	5001.279
VO ₂ -B _{0.3}	11565.824	8233.9145	4206.58	4330.59	27722.54	1130.806
VO ₂ -B _{1.0}	17272.307	8752.8466	5591.05	4052.53	31404.20	0.09615

3. Supported Fig.s



Fig. S1. XRD pattern of VO₂ and VO₂- B_x (x = 0.05, 0.3, 1.0).



Fig. S2. H content of VO_2 and VO_2 -B_x (x = 0.01, 0.03, 0.1, 0.3, 0.5, 1.0).



Fig. S3. SEM images of (a) VO₂-B_{0.05}, (a) VO₂-B_{0.1}, (c) VO₂-B_{0.3}, (d) VO₂-B_{1.0}.







Fig. S5. HR-TEM images of pristine VO₂.



Fig. S6. SAED pattern of VO₂.



Fig. S7. TEM images of VO_2 - $B_{0.5}$.



Fig. S8. Photographs of the MoO_3 and MoO_3 -B_{0.5} by sodium borohydride grinding treatment.



Fig. S9. Ultraviolet-visible diffuse reflectance spectroscopy of MoO_3 and MoO_3 -B_{0.5}.



Fig. S10. Tauc's bandgap plot of MoO₃ and MoO₃-B_{0.5}.



Fig. S11. XRD patterns of MoO_3 and MoO_3 -B_{0.5}.



Fig. S12. The electrical conductivity of MoO₃ and MoO₃-B_{0.5}.



Fig. S13. The front views on the supercells of (a) $H_9V_{32}O_{64}$ (bulk VO₂, 14.0% H-doping), (b) $H_8V_{32}O_{63}$ (1.56% O-vacancy), (c) $H_6V_{32}O_{61}$ (4.69% O-vacancy), (d) $H_4V_{32}O_{59}$ (7.81% O-vacancy). The red balls denote V atoms, the green balls denote O atoms, and the yellow balls means H atoms.



Fig. S14. The profile views on the supercells of (a) $H_9V_{32}O_{64}$ (bulk VO₂, 14.0% H-doping), (b) $H_8V_{32}O_{63}$ (1.56% O-vacancy), (c) $H_6V_{32}O_{61}$ (4.69% O-vacancy), (d) $H_4V_{32}O_{59}$ (7.81% O-vacancy). The red balls denote V atoms, the green balls denote O atoms, and the yellow balls means H atoms.



Fig. S15. The aerival views on the supercells of (a) $H_9V_{32}O_{64}$ (bulk VO₂, 14.0% H-doping), (b) $H_8V_{32}O_{63}$ (1.56% O-vacancy), (c) $H_6V_{32}O_{61}$ (4.69% O-vacancy), (d) $H_4V_{32}O_{59}$ (7.81% O-vacancy). The red balls denote V atoms, the green balls denote O atoms, and the yellow balls means H atoms.



Fig. S16. The stereochemical structures of (a) $H_9V_{32}O_{64}$ (bulk VO₂, 14.0% H-doping), (b) $H_8V_{32}O_{63}$ (1.56% O-vacancy), (c) $H_6V_{32}O_{61}$ (4.69% O-vacancy), (d) $H_4V_{32}O_{59}$ (7.81% O-vacancy). The red balls denote V atoms, the green balls denote O atoms, and the yellow balls means H atoms.



Fig. S17. Tauc's bandgap plot of VO_2 and VO_2 -B_{0.5}.



Fig. S18. Simulated density of states (DOS) of V atoms with $H_9V_{32}O_{64}$, $H_8V_{32}O_{63}$, $H_6V_{32}O_{61}$ and $H_4V_{32}O_{59}$ with different content of Oxygen vacancy in the lattice, shaded areas (S1 = 33.47, S2 = 34.63, S3 = 35.44, S4 = 37.14).



Fig. S19. The reflection loss curves of VO₂ with a sample thickness of (a) 1.9 mm and (b) 2.3 mm.



Fig. S20. The reflection loss curves of VO_2 -B_{0.05} with a sample thickness of (a) 2.7 mm and (b) 1.6 mm.



Fig. S21. The reflection loss curves of VO_2 -B_{0.1} with a sample thickness of (a) 2.9 mm and (b) 2.4 mm.



Fig. S22. The reflection loss curves of VO_2 -B_{0.3} with a sample thickness of (a) 2.1 mm and (b) 1.9 mm.



Fig. S23. The reflection loss curves of VO_2 -B_{0.5} with a sample thickness of (a) 2.0 mm and (b) 1.5 mm.



Fig. S24. The reflection loss curves of VO_2 -B_{1.0} with a sample thickness of (a) 1.4 mm and (b) 1.2 mm.



Fig. S25. EMA performance of (a, b) MoO₃, (c, d) MoO₃-B_{0.5}.



Fig. S26. The real permeability and imaginary permeability of VO₂-B_X.



Fig. S27 The magnetic loss of VO_2 and VO_2 -B_x (x= 0.05, 0.1, 0.3, 0.5, 1.0).



Fig. S28. RL vs. frequency plots of VO₂ (1.5-5.0 mm-thick).



Fig. S29. RL vs. frequency plots of VO₂-B_{0.05} (1.5-5.0 mm-thick).



Fig. S30. RL vs. frequency plots of VO₂-B_{0.1} (1.5-5.0 mm-thick).



Fig. S31. RL vs. frequency plots of VO₂-B_{0.3} (1.5-5.0 mm-thick).



Fig. S32. RL vs. frequency plots of VO_2 - $B_{0.5}$ (1.5-5.0 mm-thick).



Fig. S33. The impedance values of VO_2 -B_x (x= 0.05, 0.1, 0.3, 0.5, 1.0).



Fig. S34. RL vs. frequency plots of VO_2 - $B_{1.0}$ (1.5-5.0 mm-thick).