

Supporting Information

2D Vanadium Doped Manganese Dioxides Nanosheets for Pseudocapacitive Energy Storage

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1. Morphology structure and electrochemical characterizations on β -MnO₂ (sample MO)

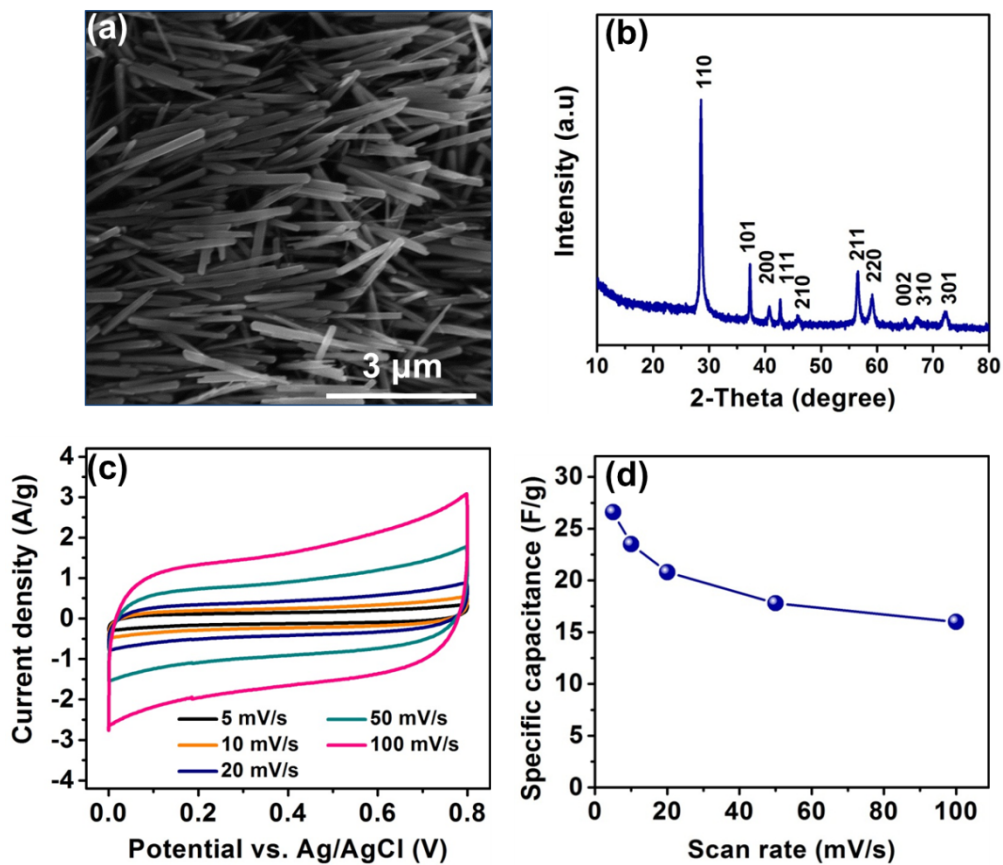


Fig. S1 (a) SEM image of β -MnO₂ (sample MO). (b) XRD pattern of β -MnO₂. (c) CV curves of β -MnO₂ at scan rate increase from 5 mV/s to 100 mV/s by a typical three-electrode configuration. (d) Gravimetric capacitance as a function of current density for β -MnO₂.

2. Morphology structure of sample 0.125 VMO and 0.25 VMO

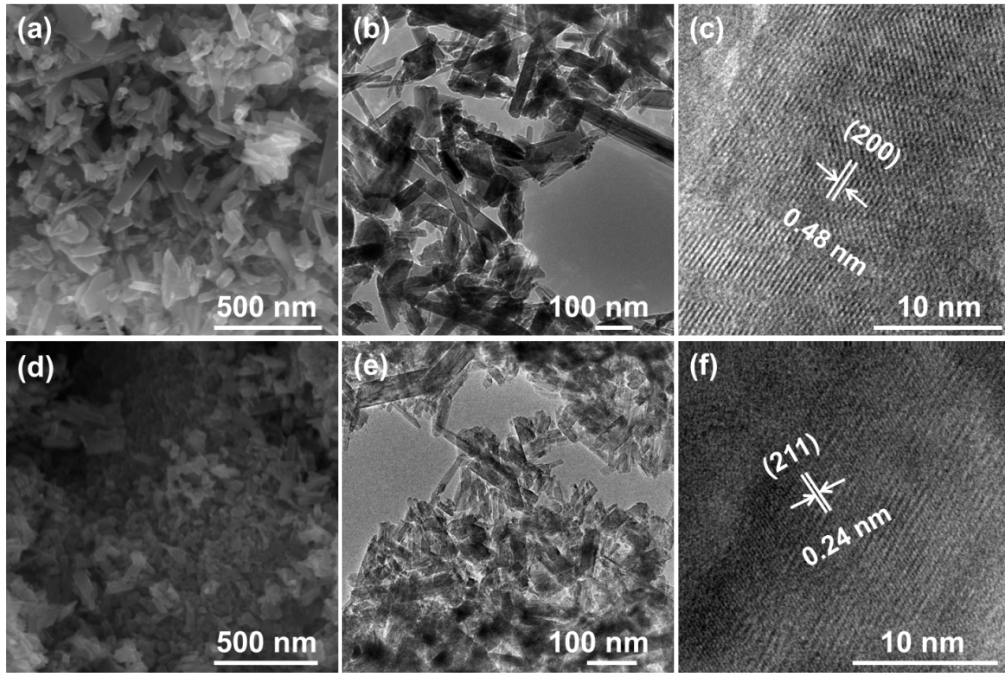


Fig. S2 (a) SEM image of sample 0.125 VMO. (b), (c) TEM and HRTEM images of sample 0.125 VMO. (d) SEM image of sample 0.25 VMO. (e), (f) TEM and HRTEM images of sample 0.25 VMO.

3. More characterizations on the V doped MnO₂ nanosheets

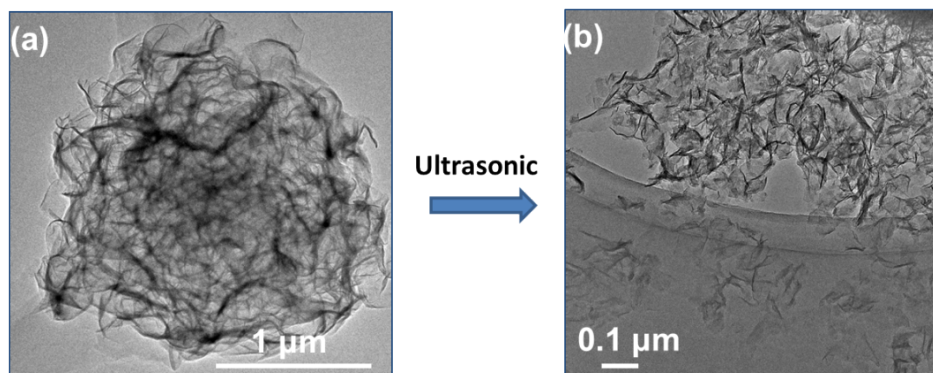


Fig. S3 (a) TEM image of sample 0.5 VMO before ultrasonic. (b) TEM image of sample 0.5 VMO after ultrasonic in ethanol and H₂O mixture solution (v:v=3:7).

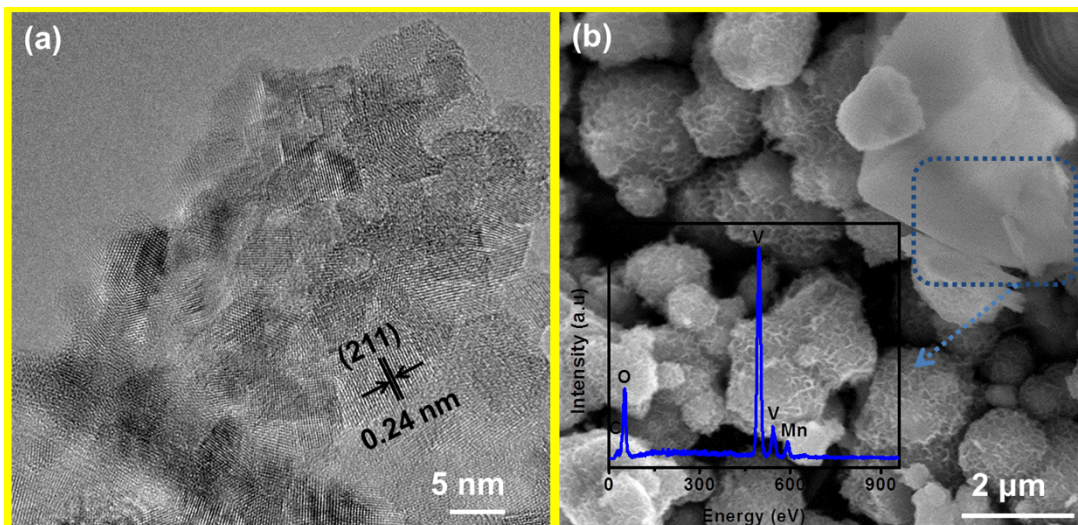


Fig. S4 (a) HRTEM image of sample 0.5 VMO. (b) SEM image of sample with a V dopant amount at 1mmol in the reaction solution, the insert shows the EDX.

Table S1: The content of element V with different test methods

Sample	Content of element V with different test methods		
	EDS	ICP-OES	XPS
0.125 VMO	1.3 (%)	1.5 (%)	1.5 (%)
0.25 VMO	2.9 (%)	2.3 (%)	2.4 (%)
0.5 VMO	5.1 (%)	5.6 (%)	4.8 (%)

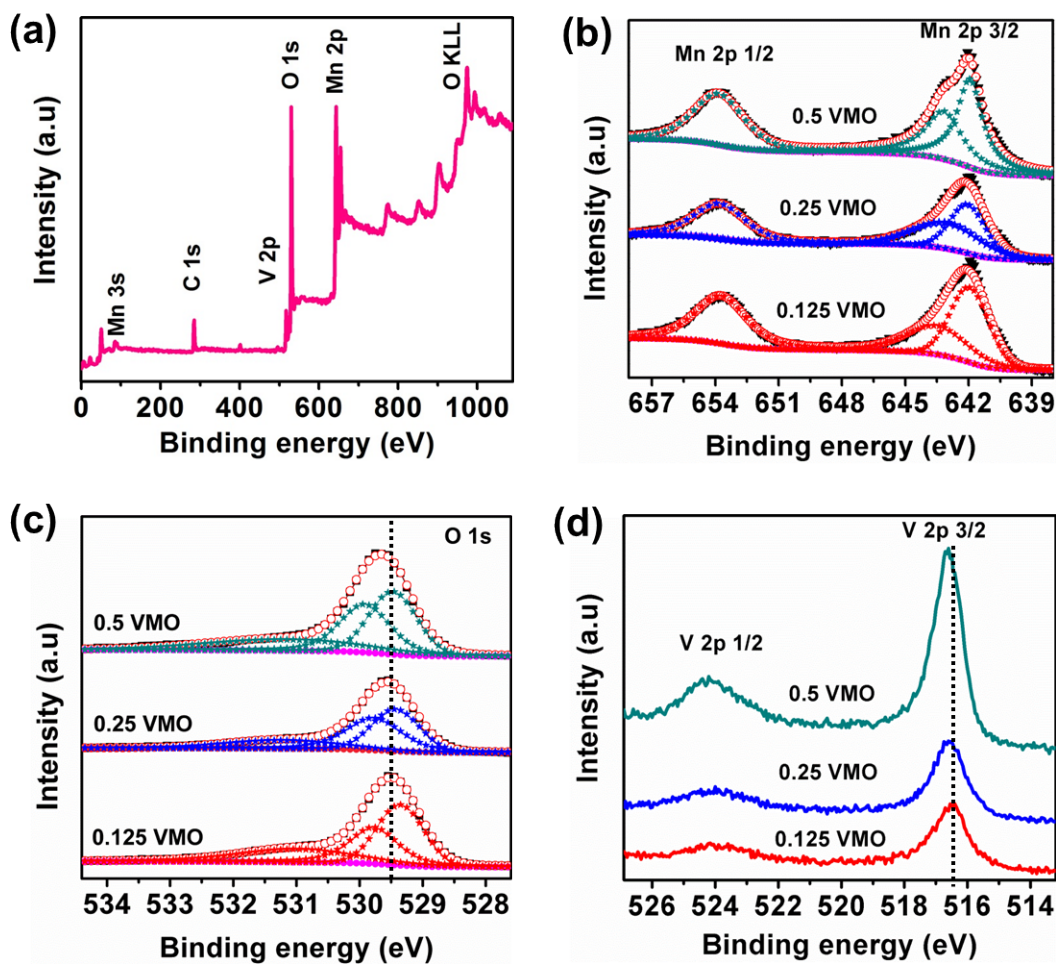


Fig. S5 (a) XPS survey spectra of sample 0.5 VMO. High-resolution XPS spectra for (b) Mn 2p, (c) O 1s, (d) V 2p of sample 0.5 VMO, 0.25 VMO, 0.125 VMO.

Table S2: Surface characteristics as derived from Nitrogen gas adsorption data

Sample	SSA (m ² /g)	Pore volume(cm ³ /g)	Pore width (nm)
0.125 VMO	92	0.368	15.9
0.25 VMO	151	0.479	12.6
0.5 VMO	273	0.670	9.0

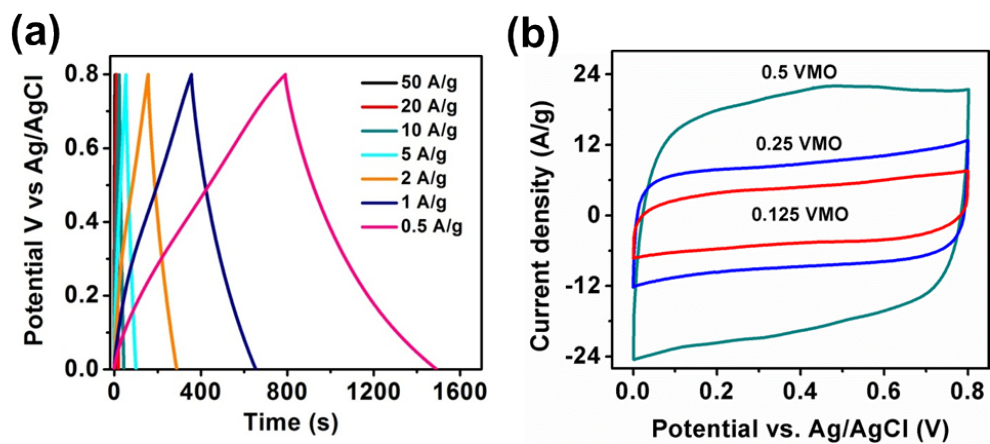


Fig. S6 (a) Galvanostatic charge/discharge curves of sample 0.5 VMO electrode with current density from 0.5 A/g to 50 A/g. (b) CV curves of sample 0.5 VMO, 0.25 VMO, 0.125 VMO at scan rate of 50 mV/s.

4. More electrochemical characterizations on the device

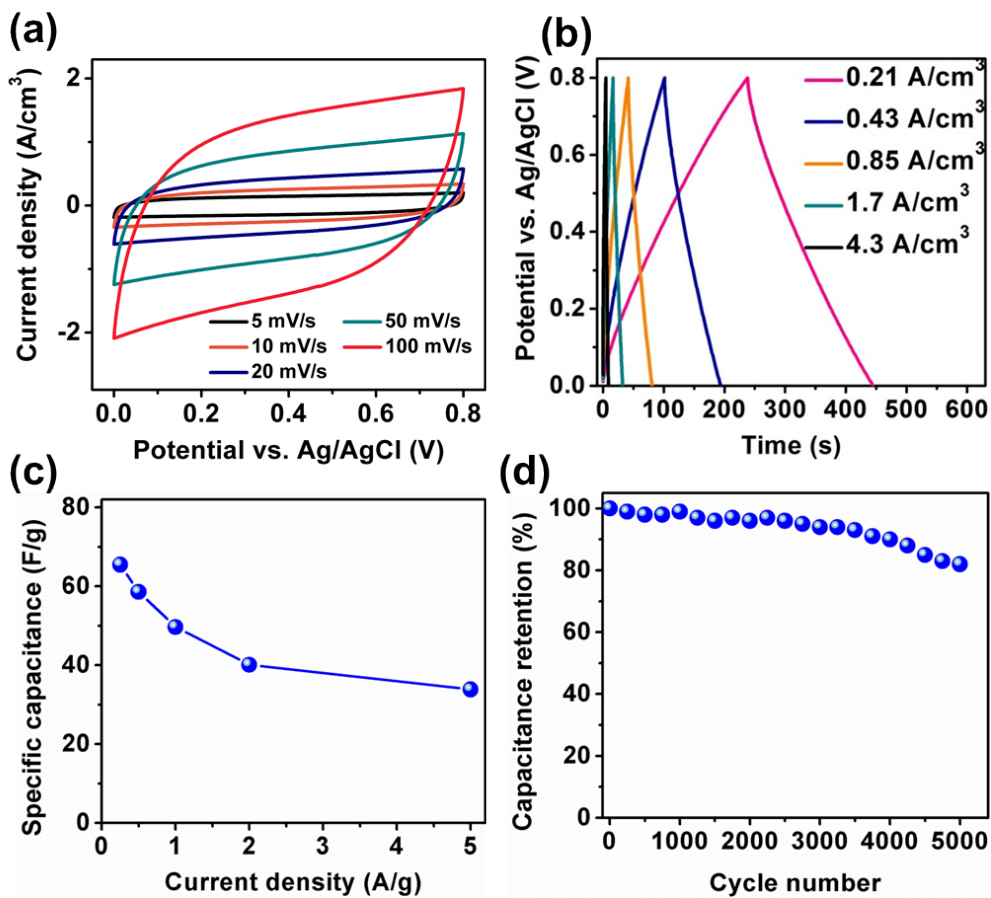


Fig. S7 (a) CV curves of the device. (b) Galvanostatic charge/discharge curves of the device. (c) Gravimetric capacitance as a function of current density for the device. (d) Cycling performance of the device.

5. Details in the first principle calculations

Our first-principle calculations are performed using VASP code ^[1] based on density-functional theory (DFT). ^[2-3]The exchange-correlation energy is described by the functional of Perdew-Burke-Ernzerhof (PBE) based on general gradient approximation (GGA) ^[4] with Hubbard U corrections (GGA+U). And in our calculations we employed GGA+U approach with $U-J = 3.9$. A plane wave cutoff of 400 eV is used. The structural relaxation is performed until the forces on all the atoms are less than 0.03 eV/Å. The brillouin zone is sampled with $2 \times 2 \times 1$ Monkhorst mesh ^[5] in structure relaxation, $4 \times 4 \times 1$ Monkhorst mesh in energy computations and $8 \times 8 \times 1$ Monkhorst mesh in density of states (DOS) computations. And spin polarization is considered in the calculations.

References

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