Supplementary Materials

Synthesis of Different Manganese Tungstate Nanostructures for Enhanced Charge Storage Application: Theoretical support of the Experimental Finding

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Table S1: Values of equivalent circuit components.

Component	Value			
Component	MWO24	MWO18	MWO12	
R ₁ (ohm)	0.51	1.18	2.36	
R ₂ (ohm)	1.01	1.34	1.50	
R ₃ (ohm)	1.55	26.97	2.99	
W ₁ (ohm S ^{-1/2})	45.49	59.7	55.22	
W ₂ (ohm S ^{-1/2})	0.86	3.01	2.24	
C ₁ (F)	0.152×10-3	1.514	0.129×10 ⁻³	
C ₂ (F)	0.117	0.079	0.912	
C ₃ (F)	0.99	2.87	0.62	

Electrode material	Electrolyte	Specific capacitance	Potential window	Cycling stability	Ref.
MnWO ₄ / RGO	6 M KOH	288 Fg ⁻¹ at 5 mV s ⁻¹	-0.35 to 0.55 V	14.9% after 6000 cycles	1
MnWO ₄	1 M Na ₂ SO ₄	386 Fg ⁻¹ at 5 mVs ⁻¹	0 to 1 V	90% after 2000 cycles	2
MnWO ₄	1 M KOH	295 Fg ⁻¹ at 5 mVs ⁻¹	-0.2 to 0.6 V	> 100% after 3000 cycles	3
MnWO ₄ micro flower	1 M Na ₂ SO ₄	$324 \text{ Fg}^{-1} \text{ at}$ 1 mA cm ⁻²	0 to 1 V	93% after 8000	4
MnWO ₄ (using DNA _scaffold)	0.1 M Na ₂ SO ₄	34 Fg ⁻¹ at 0.5 mA cm ⁻²	0 to 1 V	-	5
MnWO4 (using CTAB)	1 M H ₂ SO ₄	27 Fg ⁻¹ at 5 mVs ⁻¹ and 16 Fg ⁻¹ at 1.3 mA cm ⁻²	-0.2 to 1 V and 0 to 1 V	increased after 1000 cycles	6
MnWO ₄ @ aCNT	1 M KOH	542.18 Fg ⁻¹ at 2 mVs ⁻¹	-0.1 to 0.6 V	Above 100% after 15,000 cycles	7
MnWO ₄	0.1 M NaOH	199 Fg ⁻¹ at 2 mVs ⁻¹	0 to 0.5 V	62% after 1200 cycles	8
WO ₃ - RGO composite	0.5 M H ₂ SO ₄	495 Fg ⁻¹ at 1 Ag ⁻¹	-0.4 to 0.3 V	87.5% after 1000 cycles	9
WO ₃	0.5 M H ₂ SO ₄	319.26 Fg ⁻¹ at 0.7 Ag ⁻¹	-0.41 to 0 V	83.2% after 6000 cycles	10
WO ₃	1 M Na ₂ SO ₄	266 Fg ⁻¹ at 10 mVs ⁻¹	-0.7 to 0.4 V	81% after 1000 cycles	11
WO ₃ - WO ₃ ·0.5 H ₂ O	0.5 M H ₂ SO ₄	290 Fg ⁻¹ at 25 mVs ⁻¹	-0.6 to 0.2 V	72% after 100 cycles	12
MnWO ₄	КОН	455.07 Fg ⁻¹ at 2 mVs ⁻¹	-0.1 to 0.6 V	94% after 10,000 cycles	This work

 Table S2: Electrochemical performance comparison:



Fig. S1: Percentage distribution of (a) rod length and (b) rod diameter of MWO24 from TEM analysis.



Fig. S2: FESEM image of MWO24 electrode after 10000 cycles.



Fig. S3: (a) Total density of states (TDOS) for (-111) surface of MnWO₄, Partial density of state (PDOS) [(-111) surface of MnWO₄] for (b) Mn s orbital, (c) Mn p orbital, (d) Mn d orbital, (e) W s orbital, (f) W p orbital, (g) W d orbital (h) O s orbital and (i) O 2p orbital in 3D configuration. The Fermi level is indicated by the dotted line.





Fig. S4: Variation of quantum capacitance of MnWO₄ surface as a function of voltage using DFT D3-BJ method.

Fig. S5: (a) Total density of states (TDOS) for (-111) surface of MnWO₄, Partial density of state (PDOS) [(-111) surface of MnWO₄] for (b) Mn s orbital, (c) Mn p orbital, (d) Mn d orbital, (e) W s orbital, (f) W p orbital, (g) W d orbital (h) O s orbital and (i) O 2p orbital in 2D configuration (using DFT D3-BJ method). The Fermi level is indicated by the dotted line.

References

1. J. Tang, J. Shen, N. Li, and M. Ye, J. Alloys Compd., 2016, 666, 15-22.

2. J. Yesuraj, E. Elanthamilan, B. Muthuraaman, S. A. Suthanthiraraj, and J. P. Merlin, J. *Electron. Mater.*, 2019, **48**, 7239-7249.

3. F. Li, X. Xu, J. Huo, and W. Wang, Mater. Chem. Phys., 2015, 167, 22-27.

4. B. G. S. Raj, J. Acharya, M. K. Seo, M. S. Khil, H. Y. Kim, and B. S. Kim, *Int. J. Hydrog. Energy*, 2019, **44**, 10838-10851.

5. U. Nithiyanantham, S. R. Ede, T. Kesavan, P. Ragupathy, M. D. Mukadam, S. M. Yusuf, and S. Kundu, *RSC adv.*, 2014, **4**, 38169-38181.

6. S. Saranya, S. T. Senthilkumar, K. V. Sankar, and R. K. Selvan, *J. Electroceramics*, 2012, 28, 220-225.

7. K. Sardar, S. Thakur, S. Maiti, N. Besra, P. Bairi, K. Chanda, G. Majumdar, and K. K. Chattopadhyay, *Dalton Trans.*, 2021, **50**, 5327-5341.

8. K. K. Naik, A. S. Gangan, A. Pathak, B. Chakraborty, S. K. Nayak, and C. S. Rout, *ChemistrySelect*, 2017, **2**, pp.5707-5715.

9. J. Chu, D. Lu, X. Wang, X. Wang, and S. Xiong, J. Alloys Compd., 2017, 702, 568-572.

10. S. Yao, F. Qu, G. Wang, and X. Wu, J. Alloys Compd., 2017, 724, 695-702.

11. N. M. Shinde, A. D. Jagadale, V. S. Kumbhar, T. R. Rana, J. Kim, and C. D. Lokhande, *Korean J. Chem. Eng.*, 2015, **32**, 974-979.

12. K. H. Chang, C. C. Hu, C. M. Huang, Y. L. Liu, and C. I. Chang, J. Power Sources, 2011, 196, 2387-2392.