Supporting Information

Low-valence Bicomponent $(FeO)_x(MnO)_{1-x}$ Nanocrystals Embedded in Amorphous Carbon as High-Performance Anode Materials for Lithium Storage

Guiqiang Diao,[a] Muhammad-Sadeeq Balogun,*[b] Si-Yao Tong, [f] Xianzi Guo,[a] Xue Huang,[c] Yanchao Mao,[e] and Yexiang Tong*[d]

[a]School of Chemistry and Materials Engineering, Huizhou University, 516007 Huizhou, PR China..

[b]College of Materials Science and Engineering, Hunan University, Changsha, 410012 P. R. China. *E-mail: balogun@hnu.edu.cn

[c]College of Chemistry and Chemical Engineering, Zhongkai University of Agriculture and Engineering, Guangzhou, 510225, China.

[d]MOE of the Key Laboratory of Bioinorganic and Synthetic Chemistry, KLGHEI of Environment and Energy Chemistry, School of Chemistry, Sun Yat-Sen University, Guangzhou 510275 P. R. China *E-mail: chedhx@mail.sysu.edu.cn

[e]MOE Key Laboratory of Materials Physics, School of Physics and Engineering, Zhengzhou University, Zhengzhou 450001, China

[f] Zhixin High School, Guangzhou, 510080, P.R. China.

DFT Calculations

All the calculations were performed based on spin-polarized periodic density functional theory (DFT) implemented in Gaussian 09W.[1] The calculation basis set was B3LYP and the total energy convergence was set to be lower than 10^{-5} eV, and the force convergence was set to be smaller than 0.02 eV/Å. The crystal plane of V_2O_5 for DFT calculation is (001) facet and the crystal plane of C for DFT calculation is (001) facet (JCPDS no. #65-0131 for V_2O_5 and JCPDS no. #26-1080 for C).

Supporting Figures

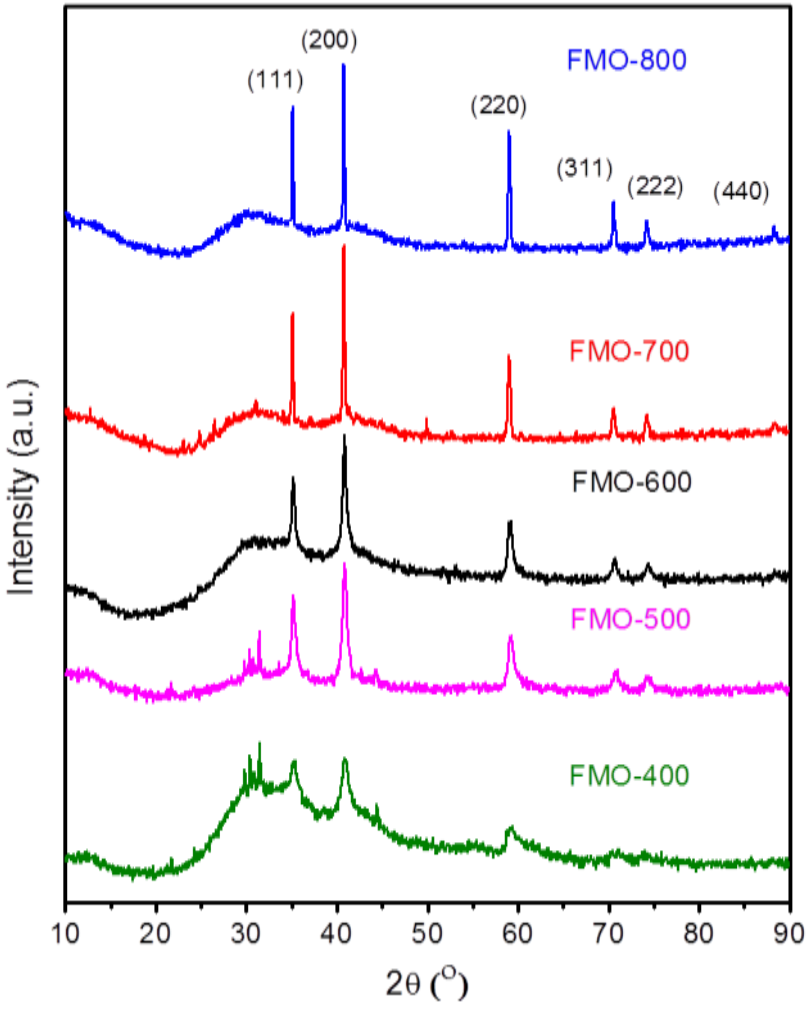

Figure S1. XRD patterns of the FMO samples at different annealing temperature from 400 °C to 800 °C.

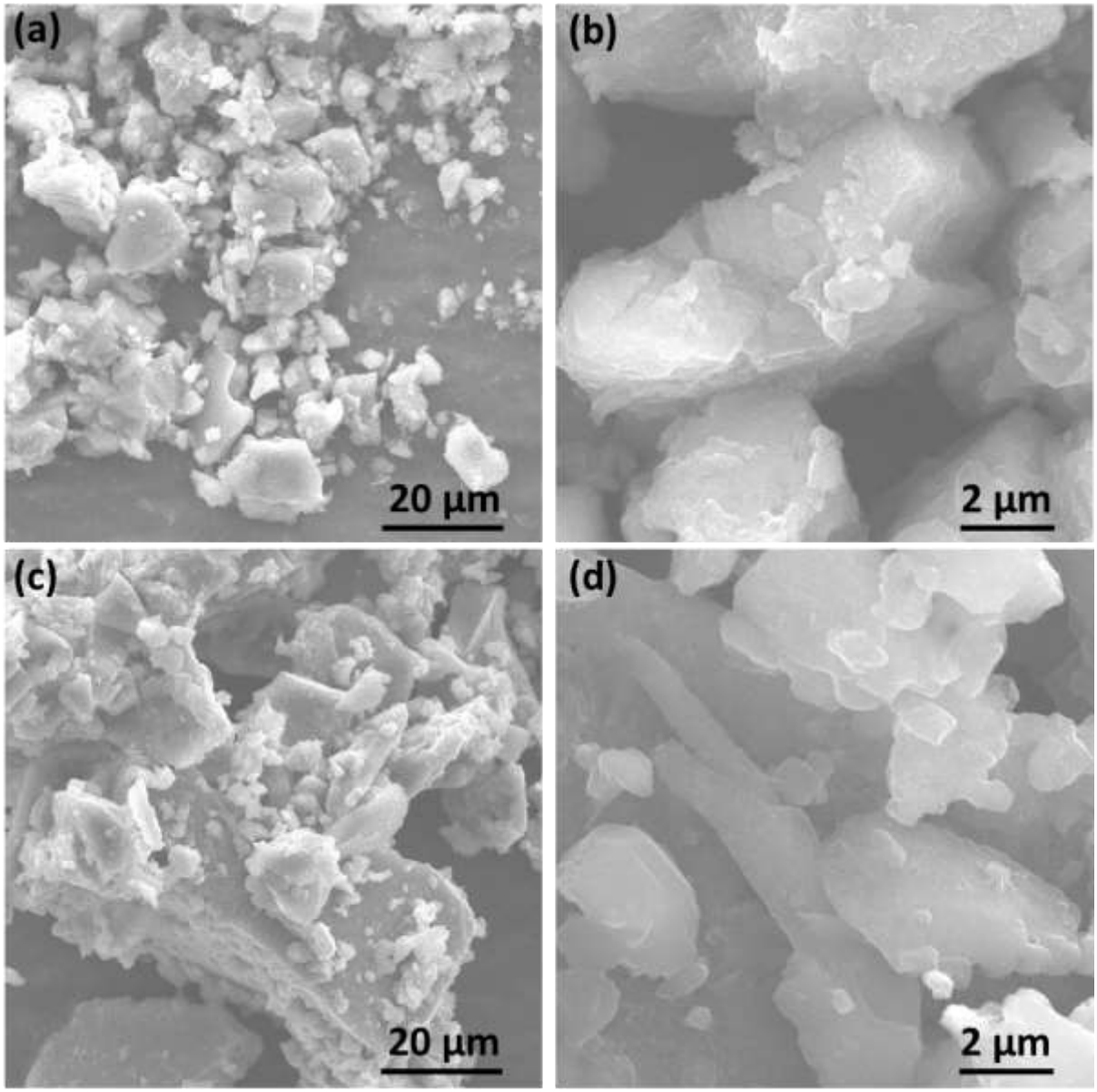

Figure S2. SEM images of (a-b) FMO-400 and (c-d) FMO-500.

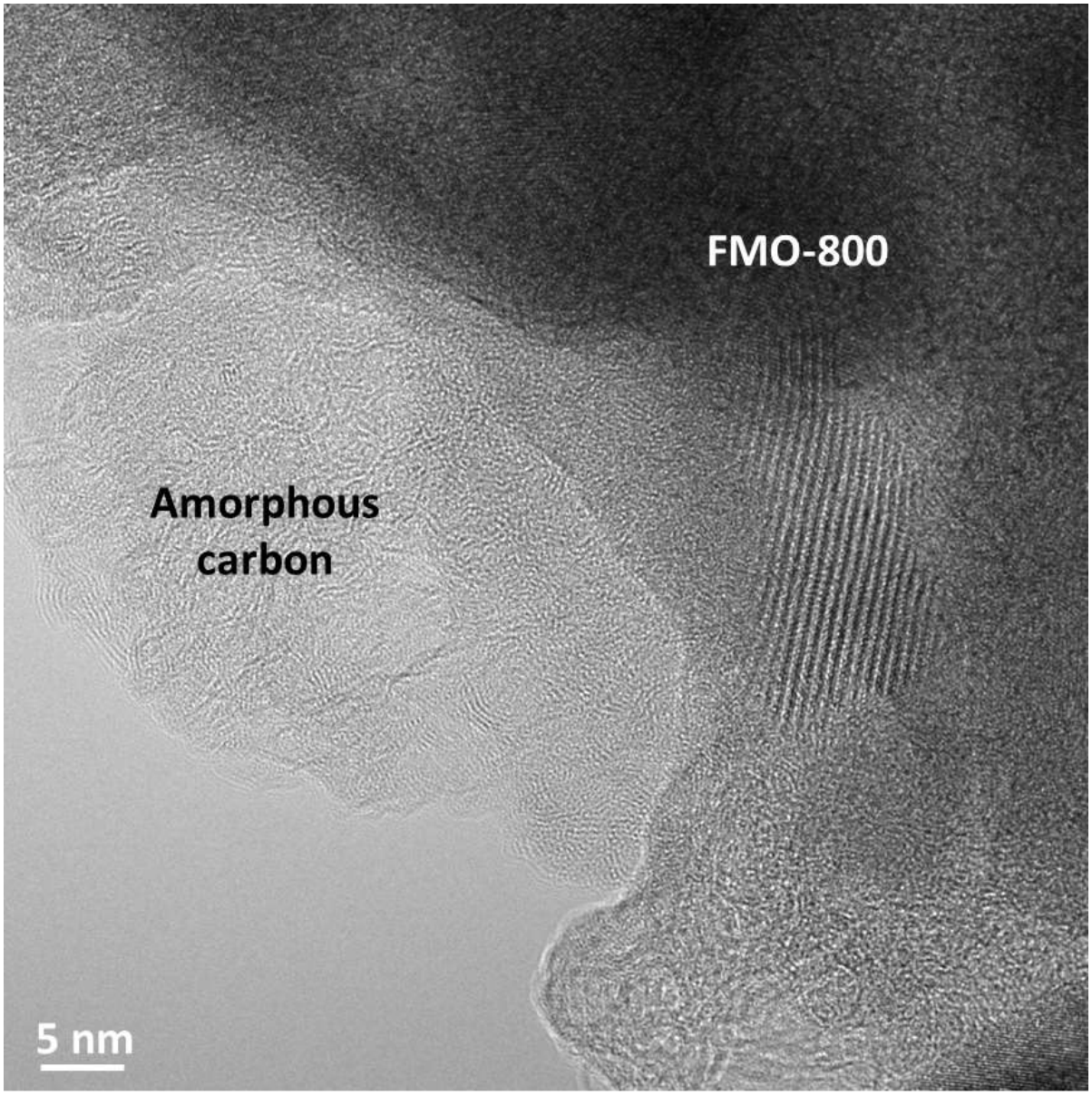

Figure S3. HRTEM of FMO-800 showing the amorphous carbon.

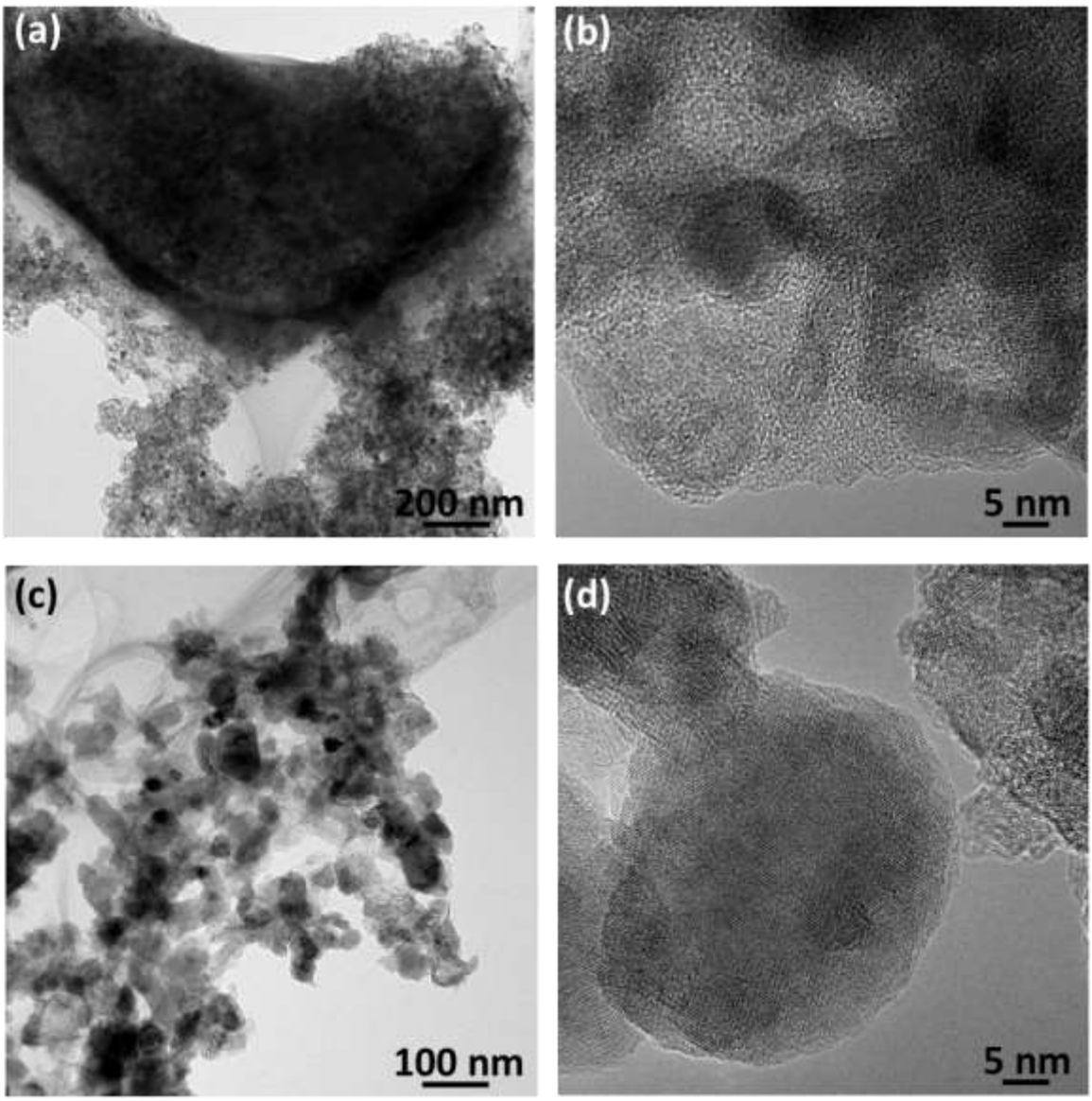

Figure S4. TEM images of (a-b) FMO-600 and (c-d) FMO-700.

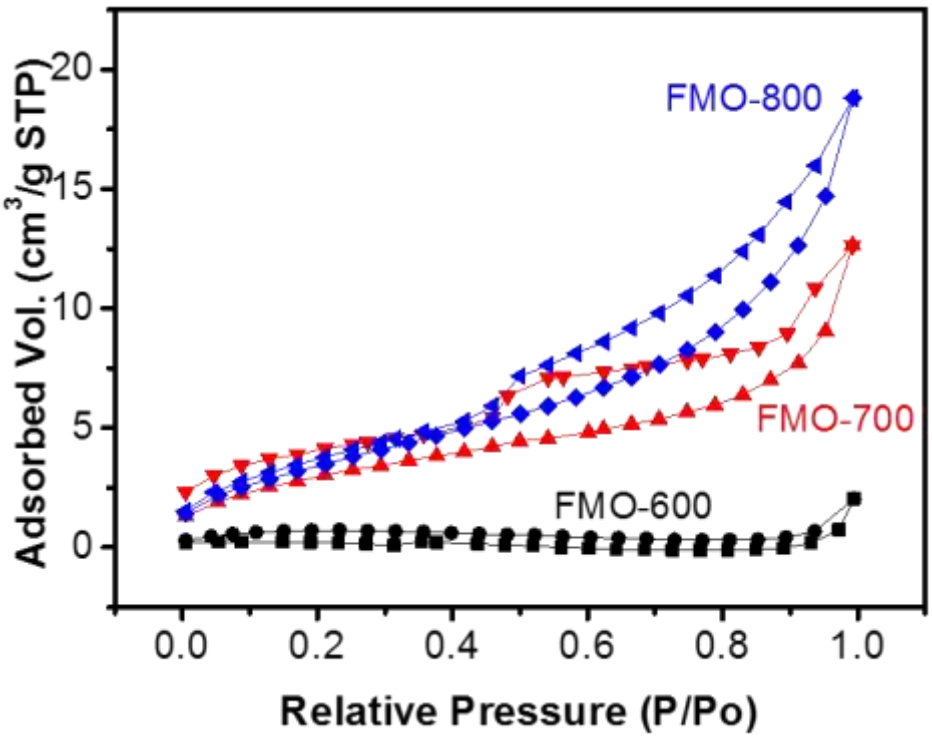

Figure S5. BET surface area of the samples.

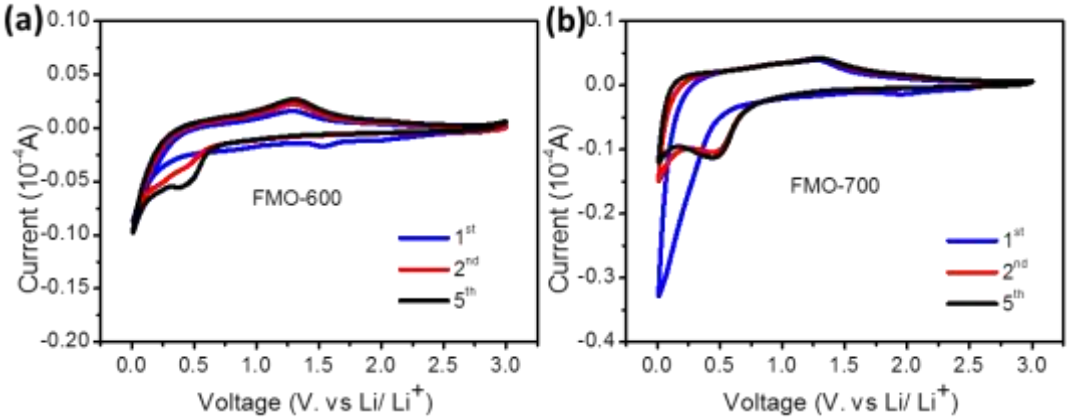

Figure S6. 1st, 2nd and 5th CV curves of (a) FMO-600 and (b) FMO-700.

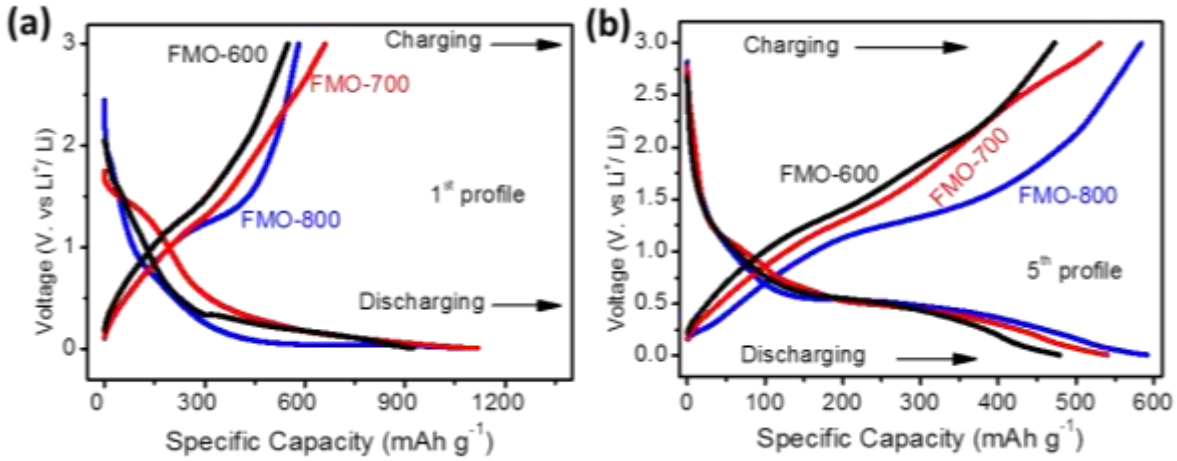

Figure S7. (a)1st and (b) 5th charge/discharge profiles of the electrodes.

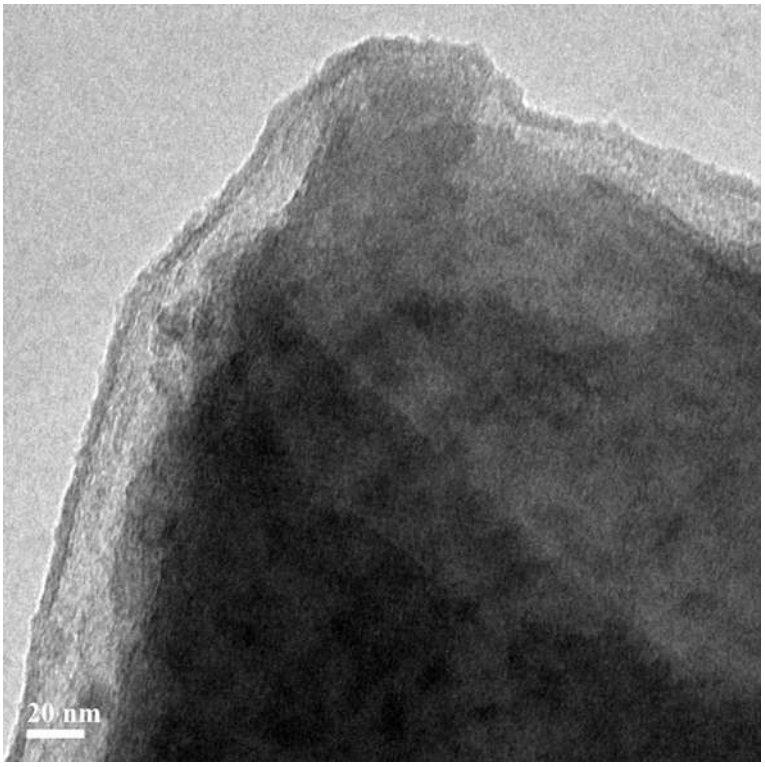

Figure S8. TEM images of FMO-800 after cyclic stability

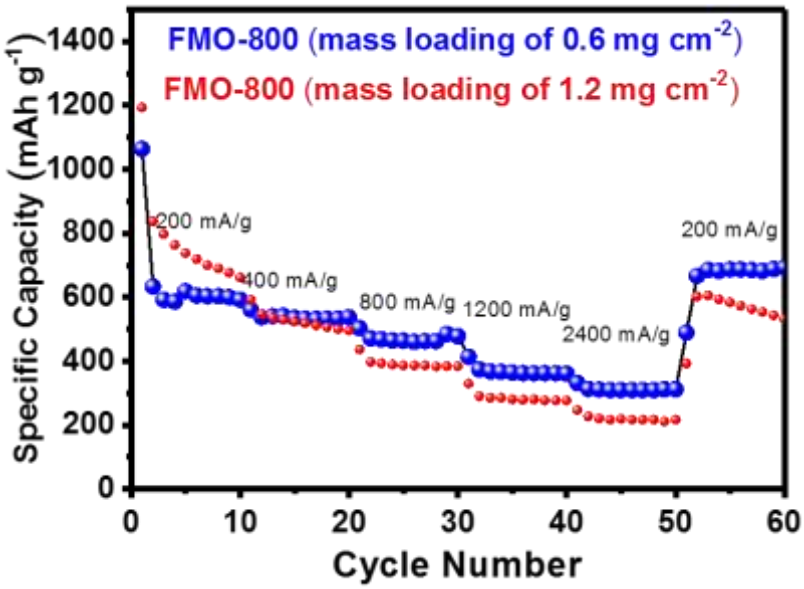

Figure S9. Rate performance of FMO-800 at different mass loading of 0.6 and 1.2 mg cm^{-2}.

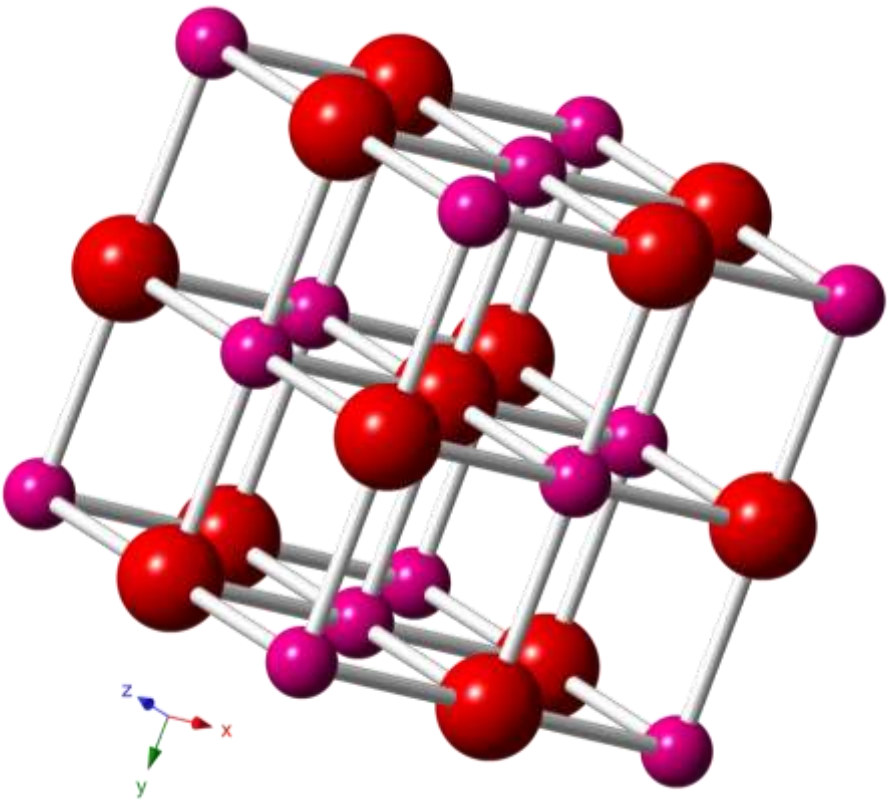

Figure S10. Optimum cluster structure of FMO-600.

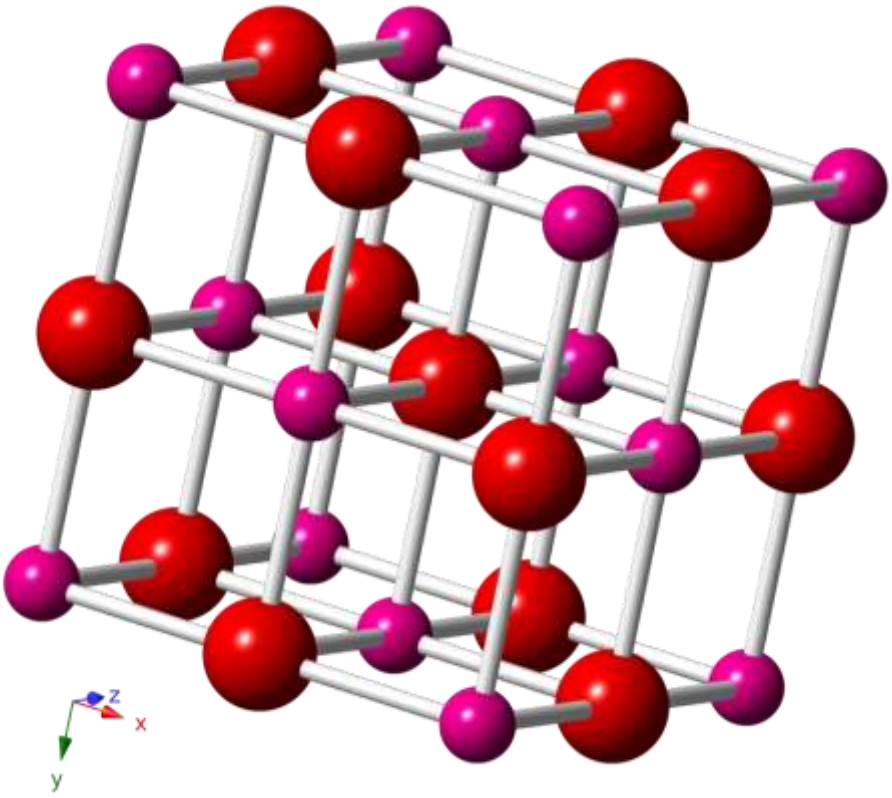

Figure S11. Optimum cluster structure of FMO-700/800.

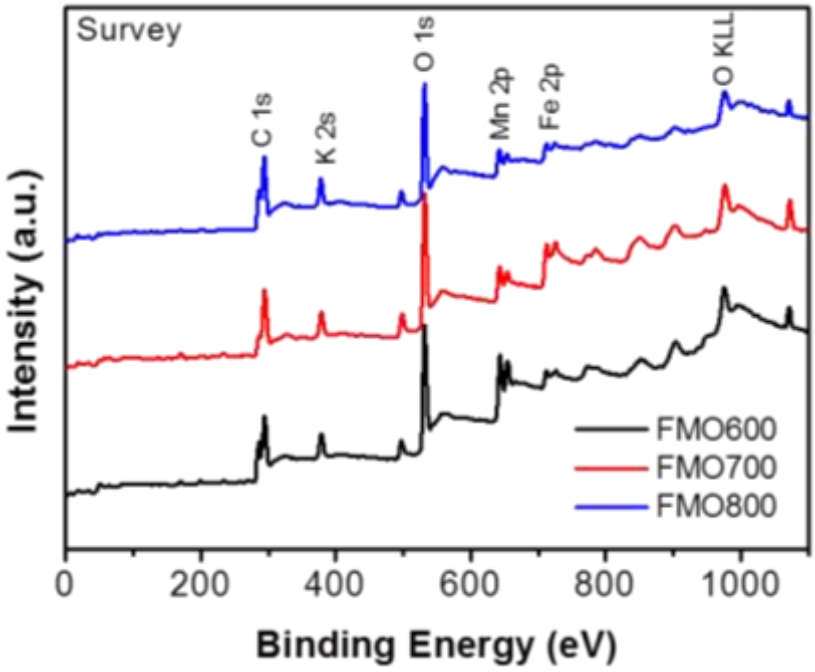

Figure S12. XPS survey spectra of the samples.

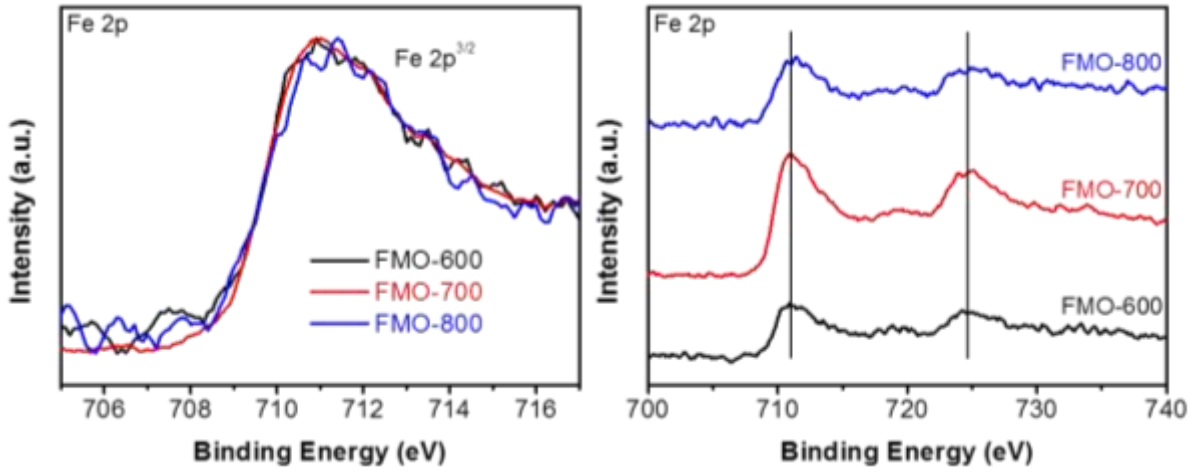

Figure S13. Fe 2p XPS survey spectra of the samples.

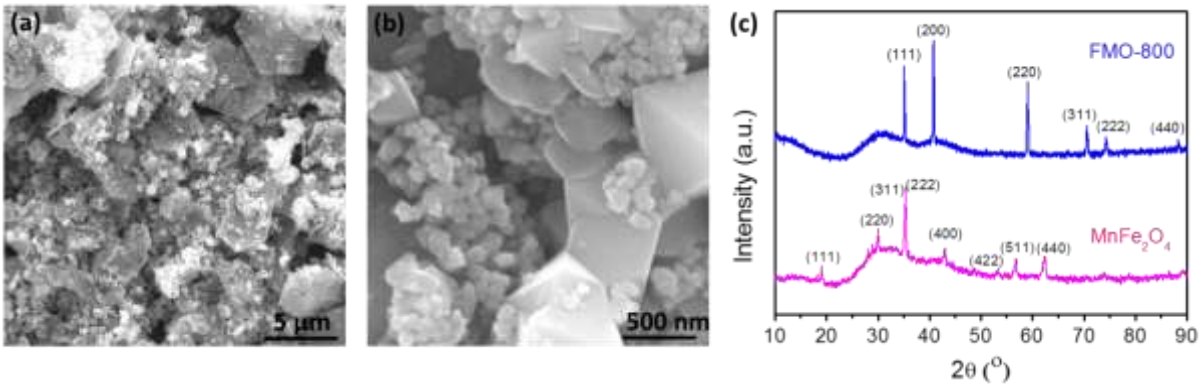

Figure S14. (a-b) SEM images of $MnFe_2O_4$. (c) XRD spectra of FMO-800 and $MnFe_2O_4$.

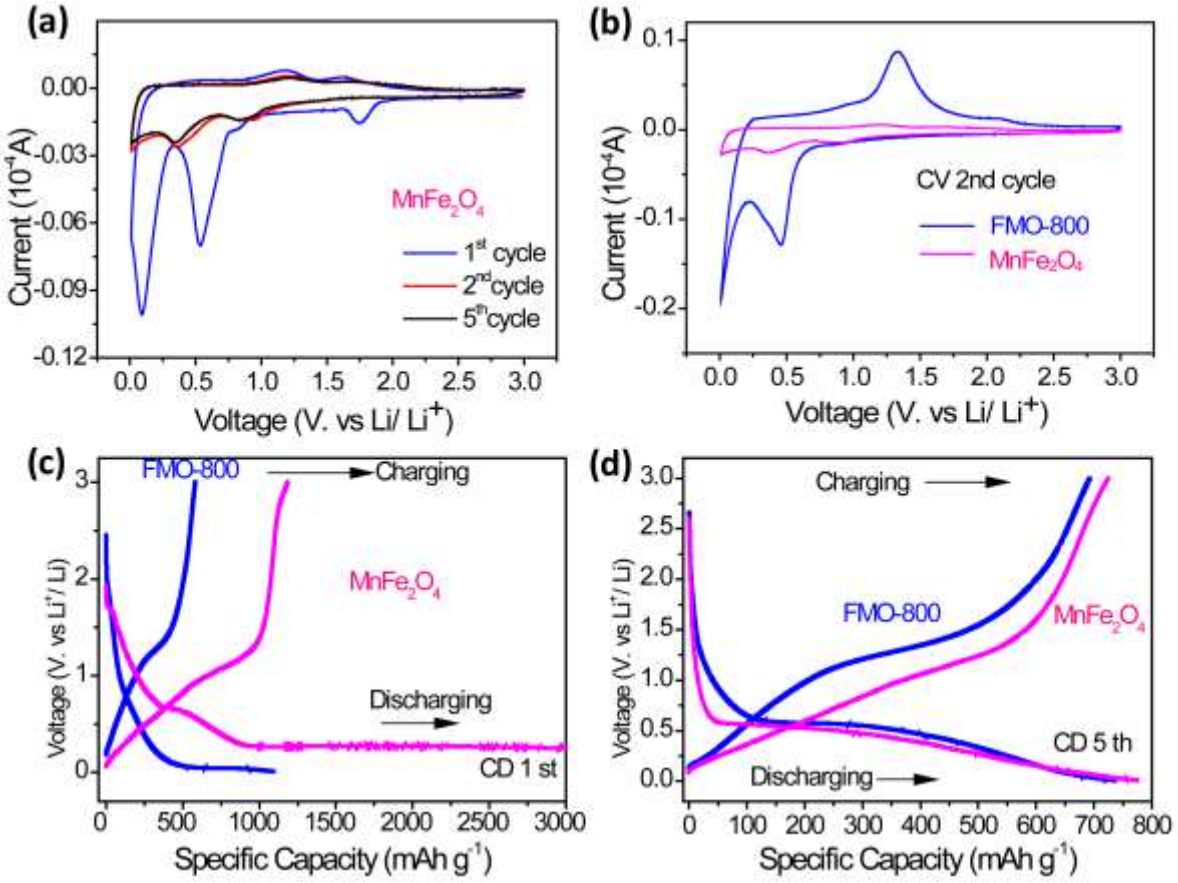

Figure S15. (a) 1st, 2nd and 5th CV curves of $MnFe_2O_4$. (b) 2nd cycle CV curves of FMO-800 and $MnFe_2O_4$. (c) 1st and (d) 5th charge/discharge profiles of FMO-800 and $MnFe_2O_4$.

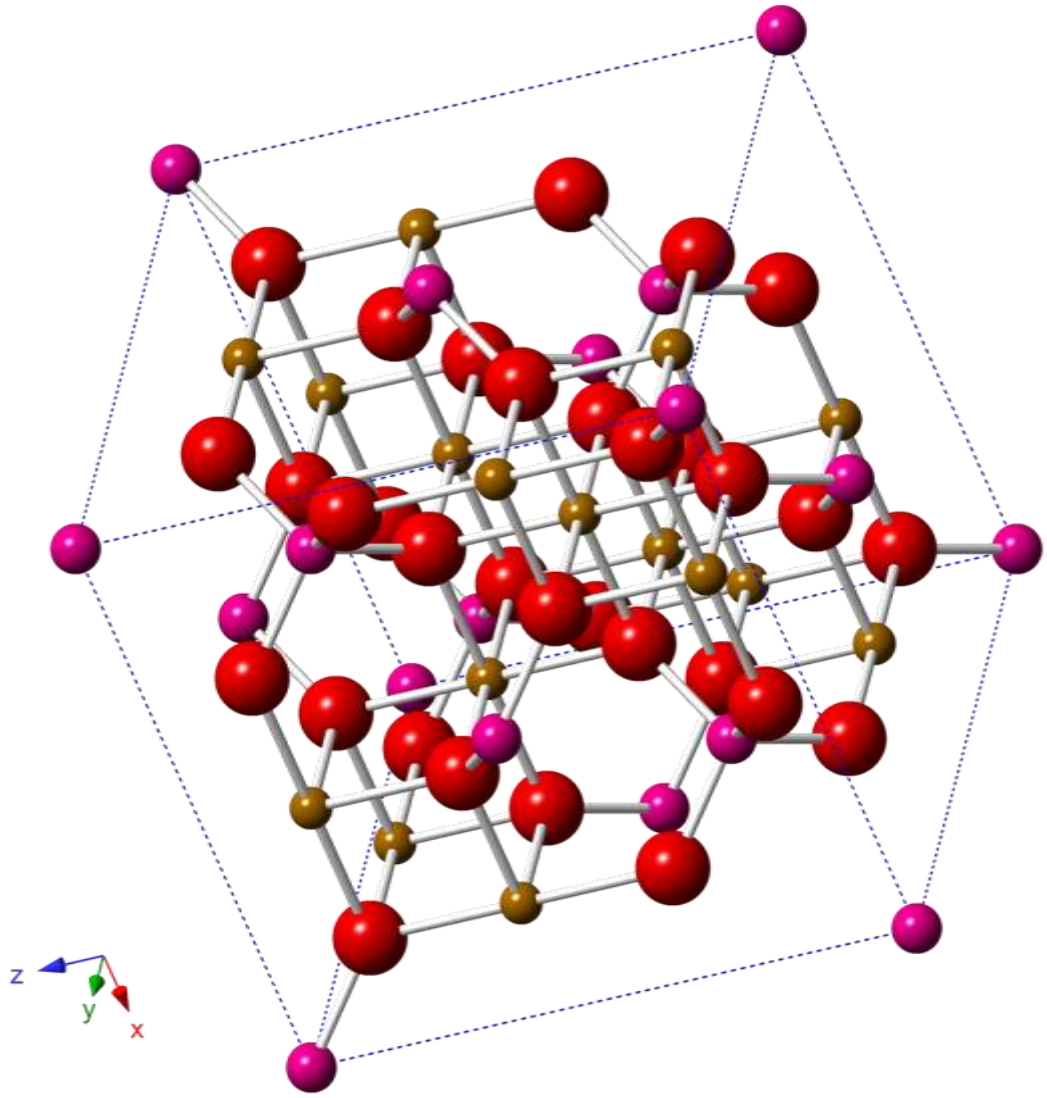

Figure S16. Optimum cluster structure of $MnFe_2O_4$.

References

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