Supplementary Information

Experimental and Theoretical Study of $LiMn_2O_4$ Synthesized by the Solution Combustion Method Using Corn Starch as Fuel

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Microstrain analysis

The Williamson-Hall method considers the line broadening as a sum of the contributions from crystallite size and microstrain. The crystallite size varies as $1/\cos\theta$ and the contribution microstrain varies as $\tan\theta$. This allows dissociating the crystallite size and microstrain contributions. The Williamson-Hall plotting to samples calcined at 500 or 700 °C using uniform deformation model (UDM), are shown in Figure S1 and the results indicate that for the sample treated at 700 °C, the slope is negative, while for the sample treated at 500 °C, the crystallite size is negative. In both cases, the information obtained has no physical meaning. Thus, the use of the conventional Williamson-Hall uniform deformation model (UDM) does not work in these samples. Other methods that incorporate the anisotropic nature of the crystal could be applied in order to extract this desired information,[1,2] but this is beyond the scope of this work.

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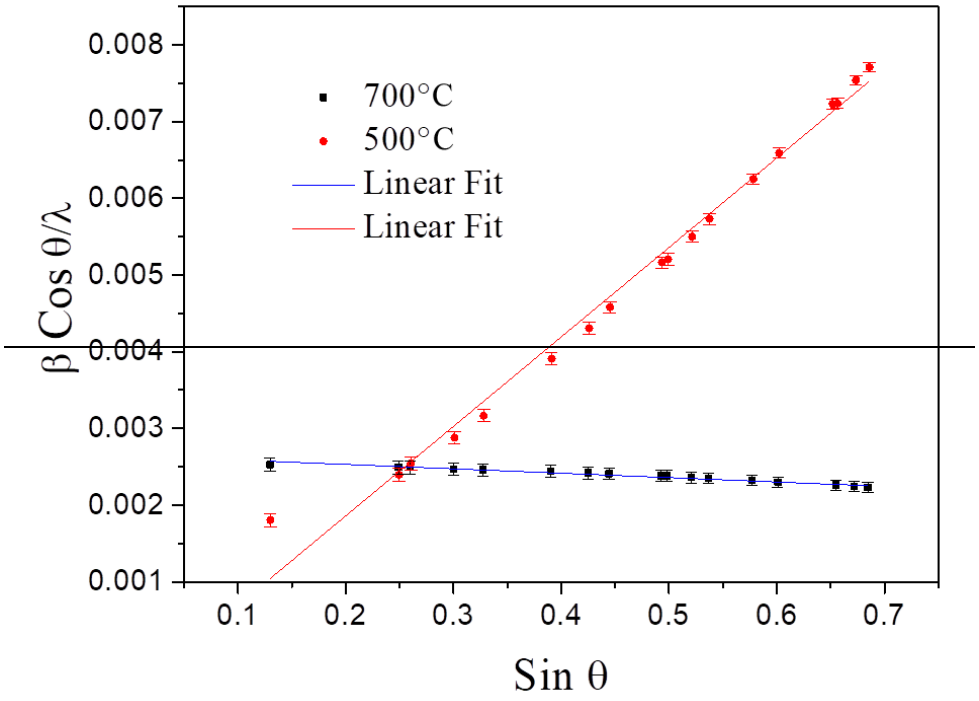

Figure S1. Williamson-Hall plotting to samples treated at 500 and 700 °C assuming the uniform deformation model.

Molecular modeling

$Mn_{16}O_{32}$

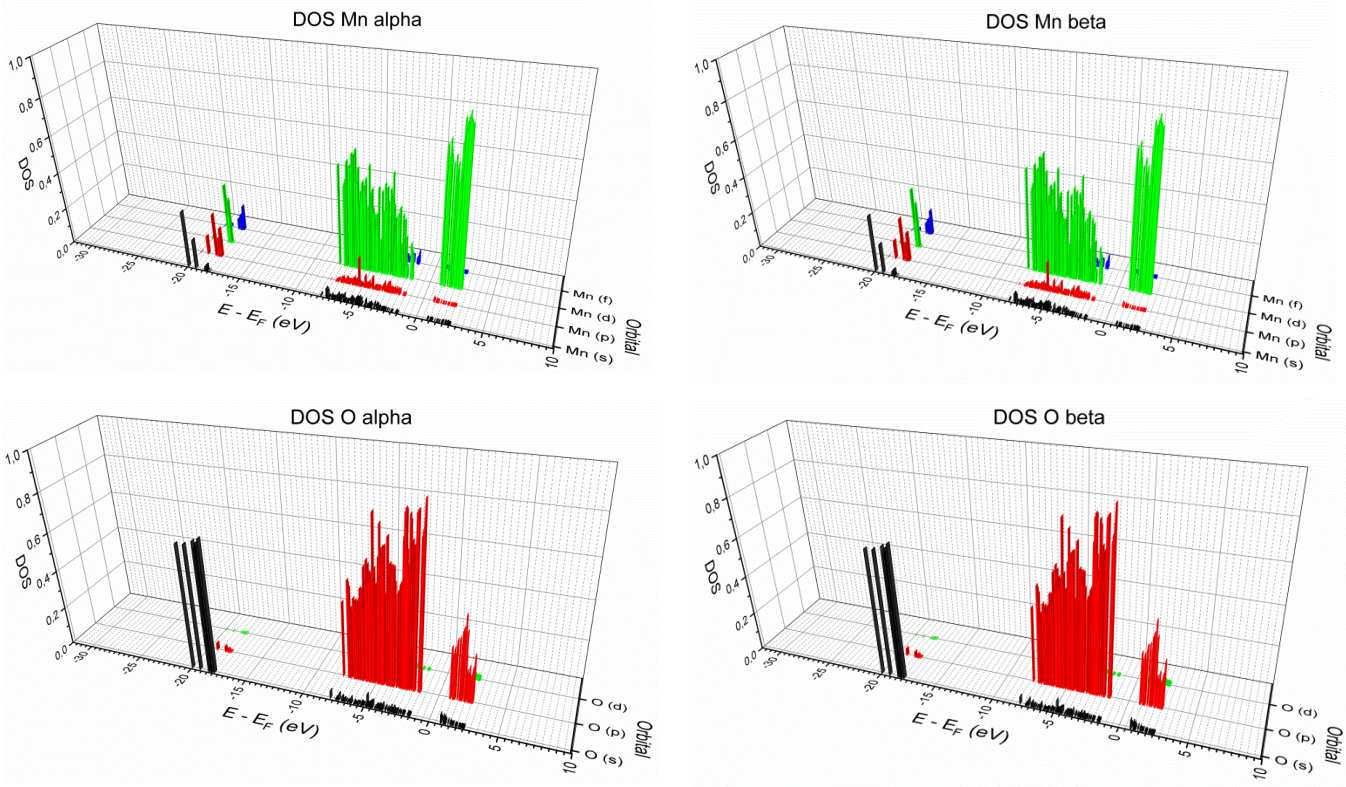

Figure S2. Density orbital state in optimized structure of $Mn_{16}O_{32}$. Method DFT/GGA, PBE-D3 functional, program CP2K, T (300 K).

$Li_2Mn_{16}O_{32}$

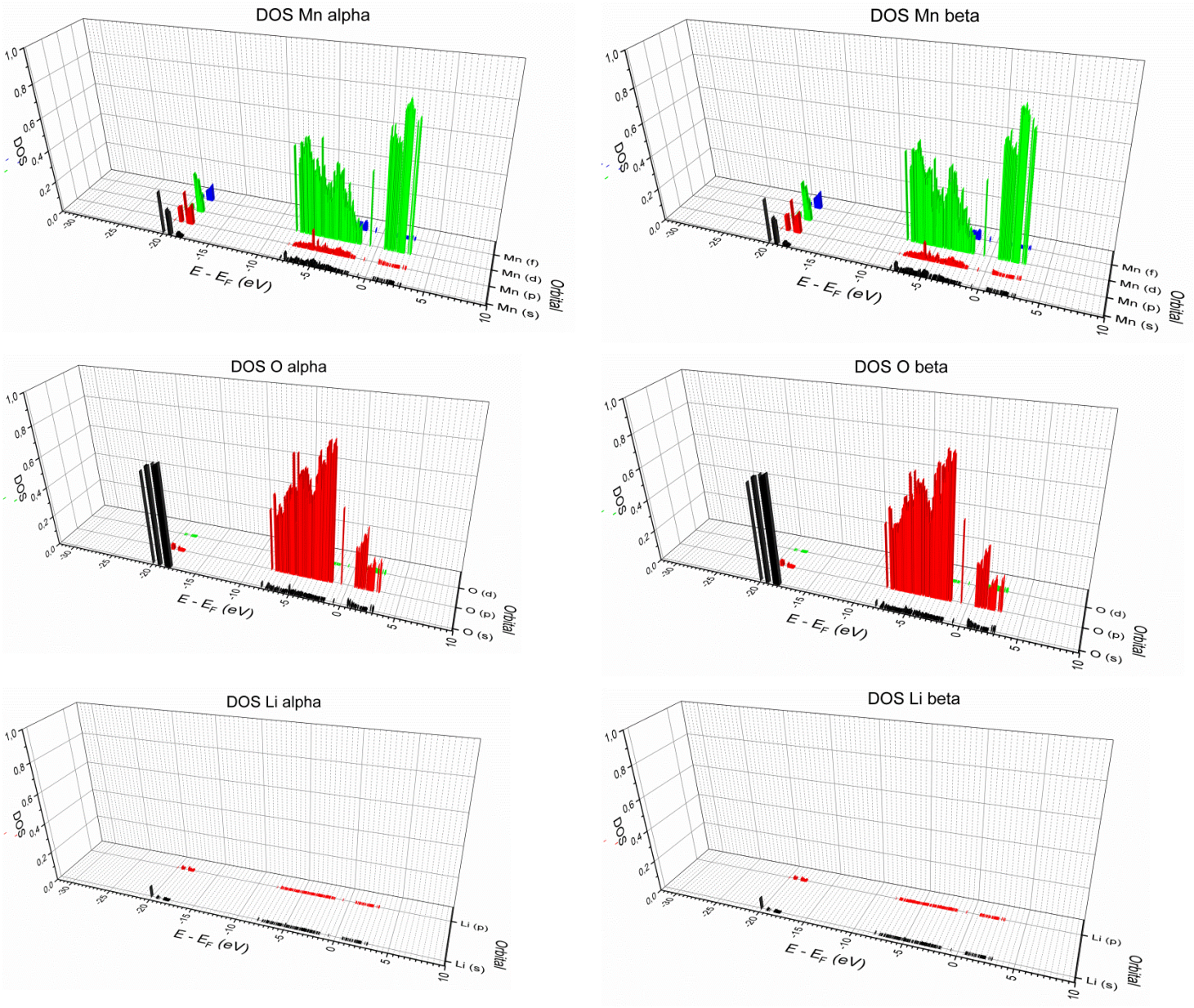

Figure S3. Density orbital state in optimized structure of $Li_2Mn_{16}O_{32}$. Method DFT/GGA, PBE-D3 functional, program CP2K, T (300 K).

$Li_4Mn_{16}O_{32}$

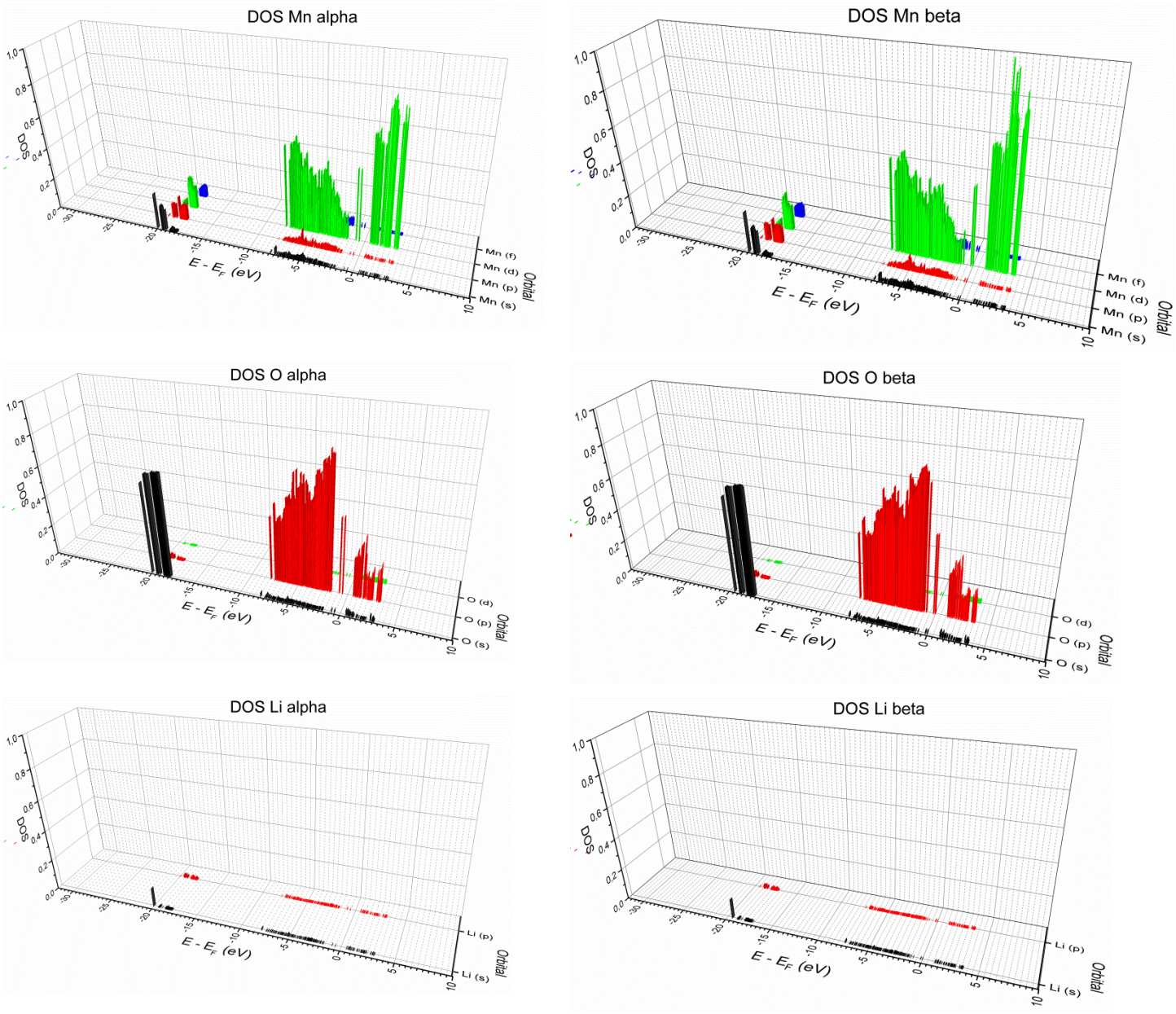

Figure S4. Density orbital state in optimized structure of $Li_4Mn_{16}O_{32}$. Method DFT/GGA, PBE-D3 functional, program CP2K, T (300 K).

$Li_6Mn_{16}O_{32}$

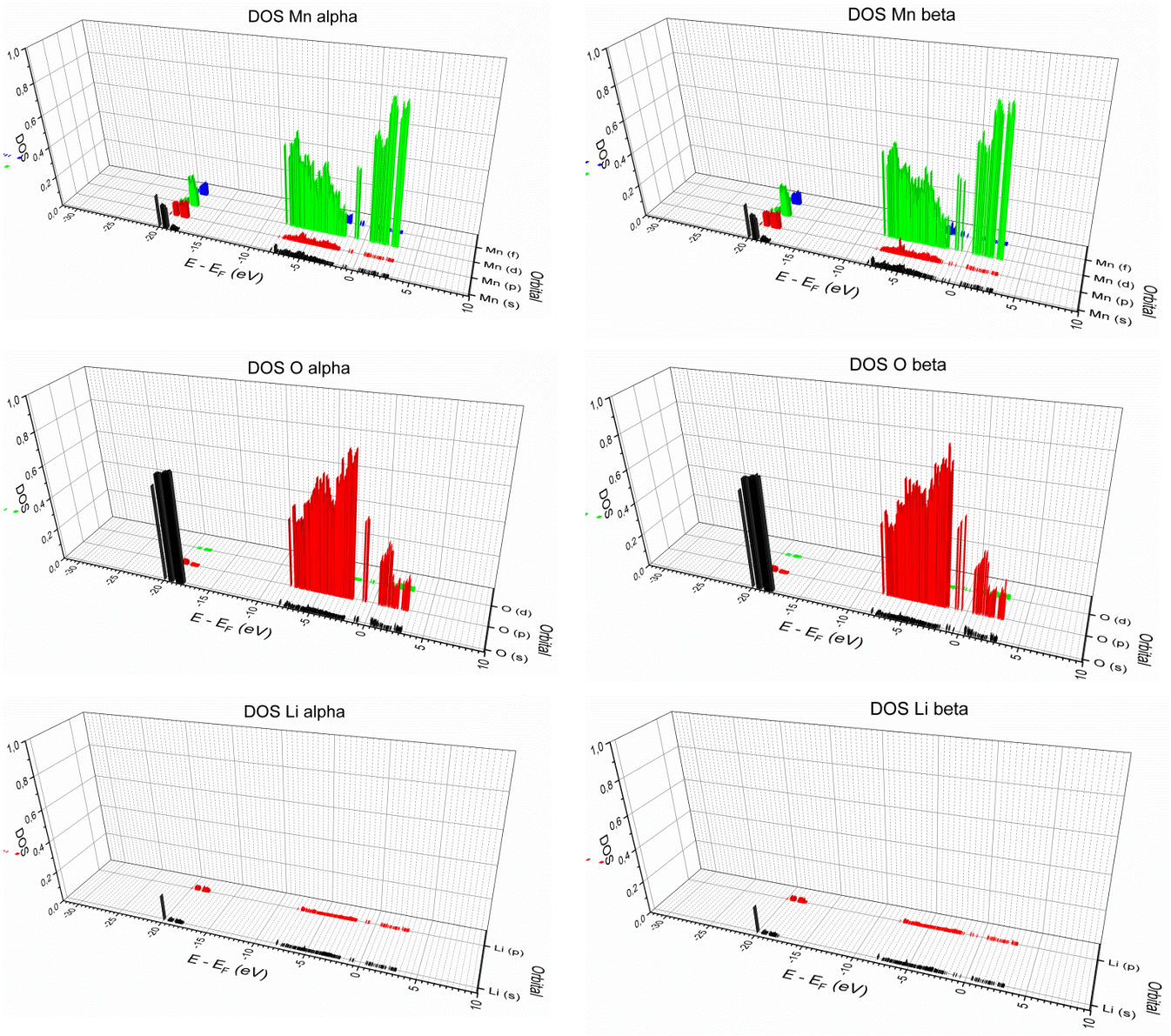

Figure S5. Density orbital state in optimized structure of $Li_6Mn_{16}O_{32}$. Method DFT/GGA, PBE-D3 functional, program CP2K, T (300 K).

$Li_7Mn_{16}O_{32}$

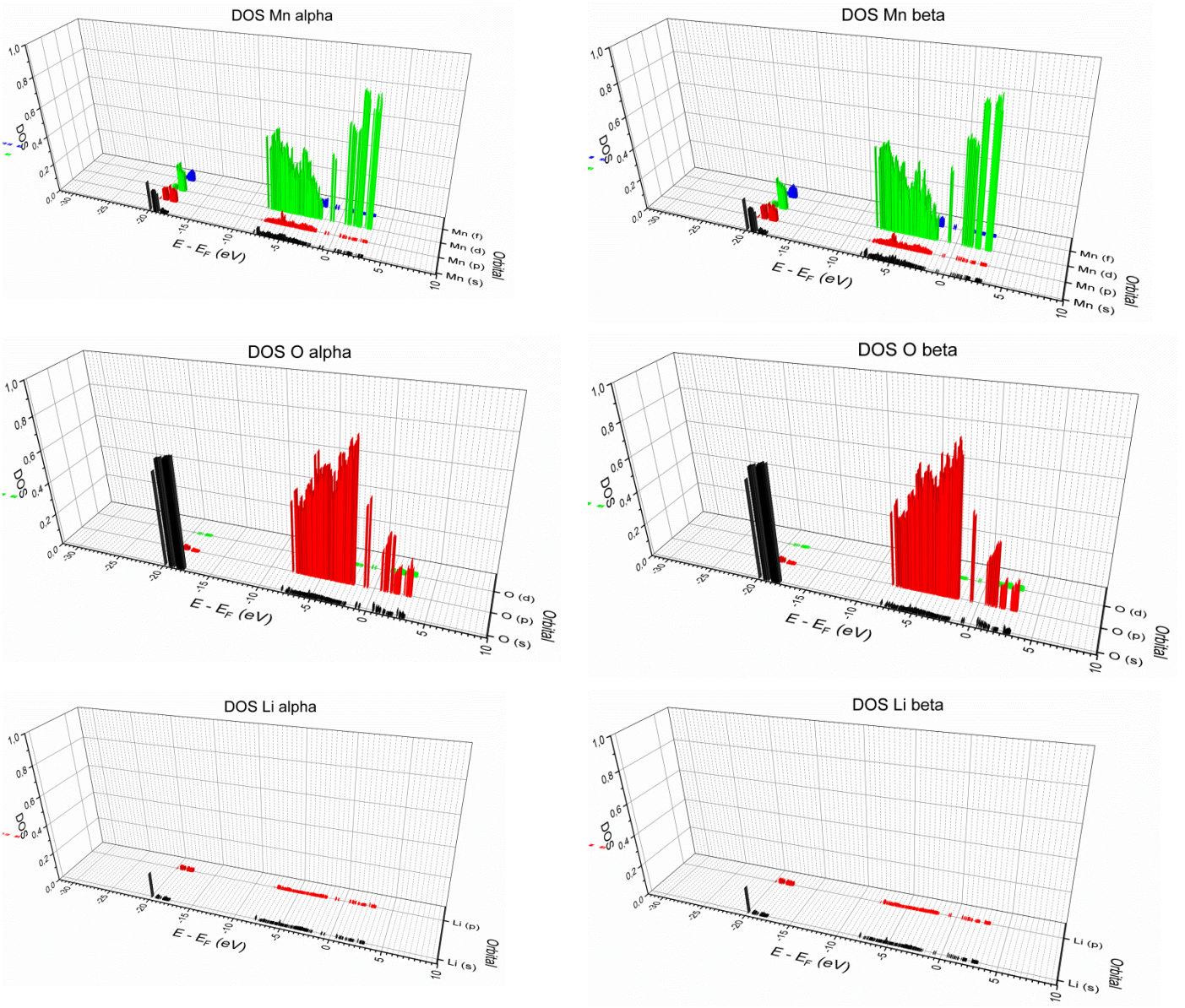

Figure S6. Density orbital state in optimized structure of $Li_7Mn_{16}O_{32}$. Method DFT/GGA, PBE-D3 functional, program CP2K, T (300 K).

$Li_8Mn_{16}O_{32}$

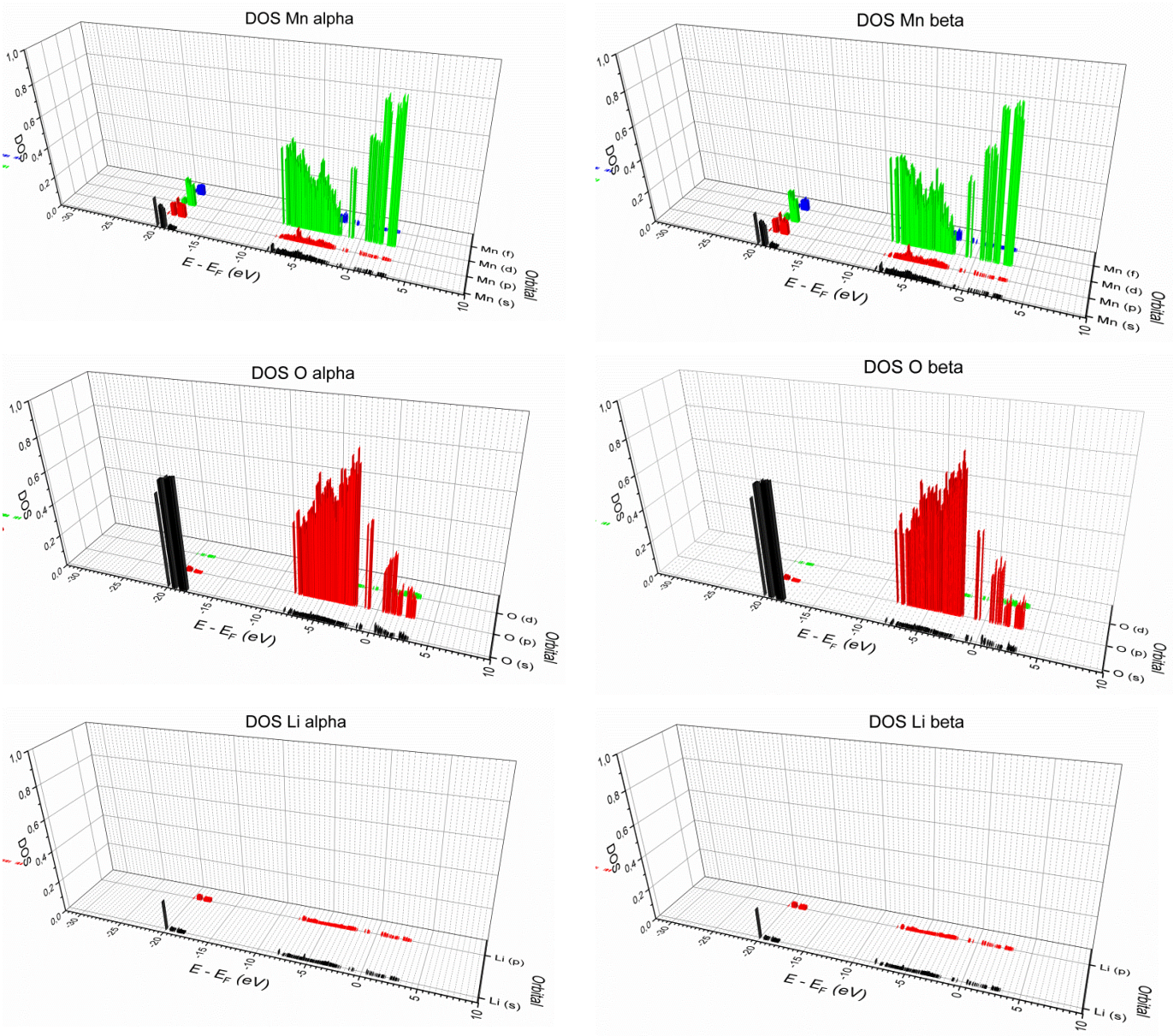

Figure S7. Density orbital state in optimized structure of $Li_8Mn_{16}O_{32}$. Method DFT/GGA, PBE-D3 functional, program CP2K, T (300 K).

$Li_8Mn_{16}O_{32}$ refined

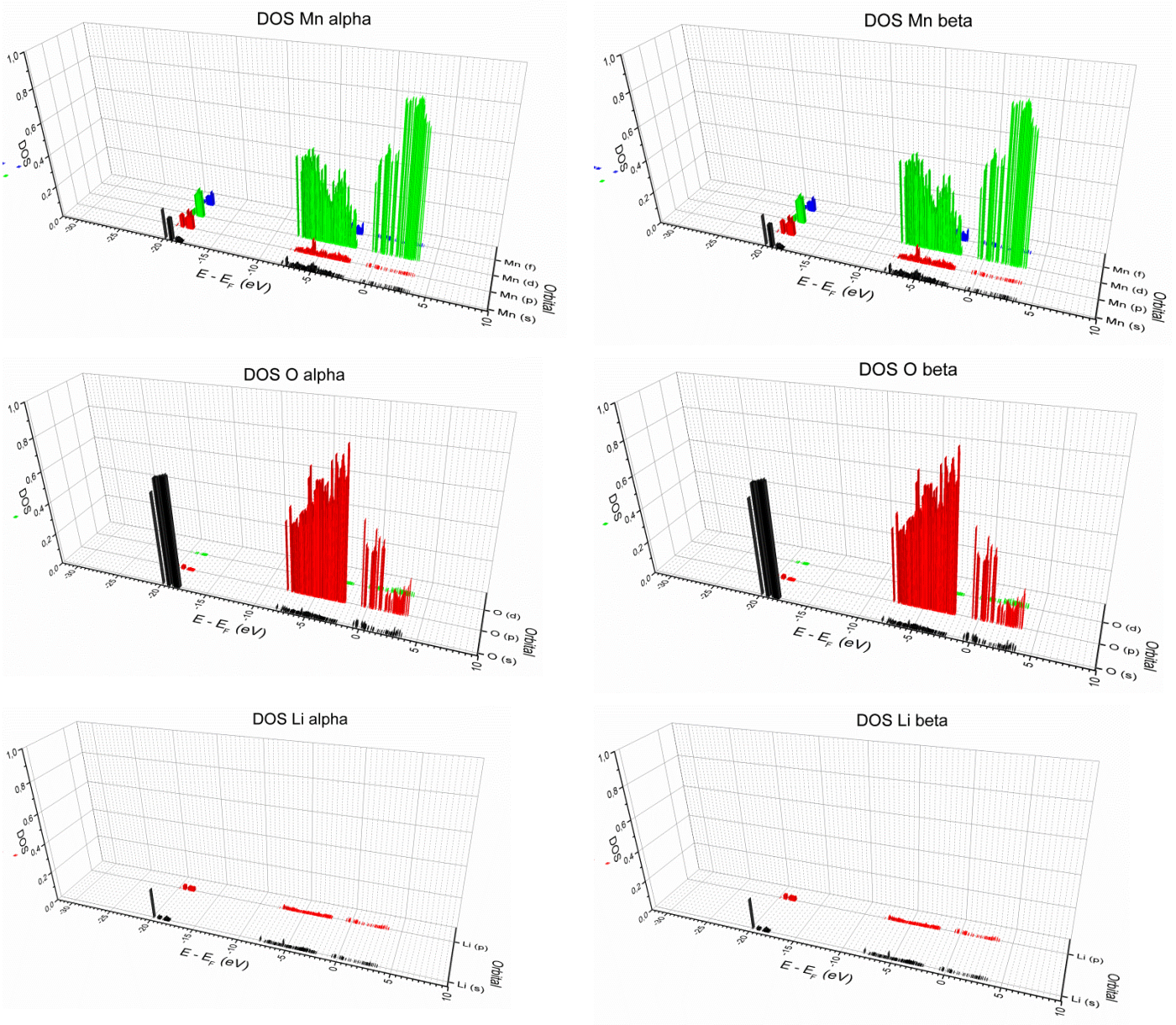

Figure S8. Density orbital state in refined structure of $Li_8Mn_{16}O_{32}$. Method DFT/GGA, PBE-D3 functional, program CP2K, T (300 K).

$Mn_{16}O_{32}$	$Li_8Mn_{16}O_{32}$
LUMO	LUMO
HOMO	HOMO

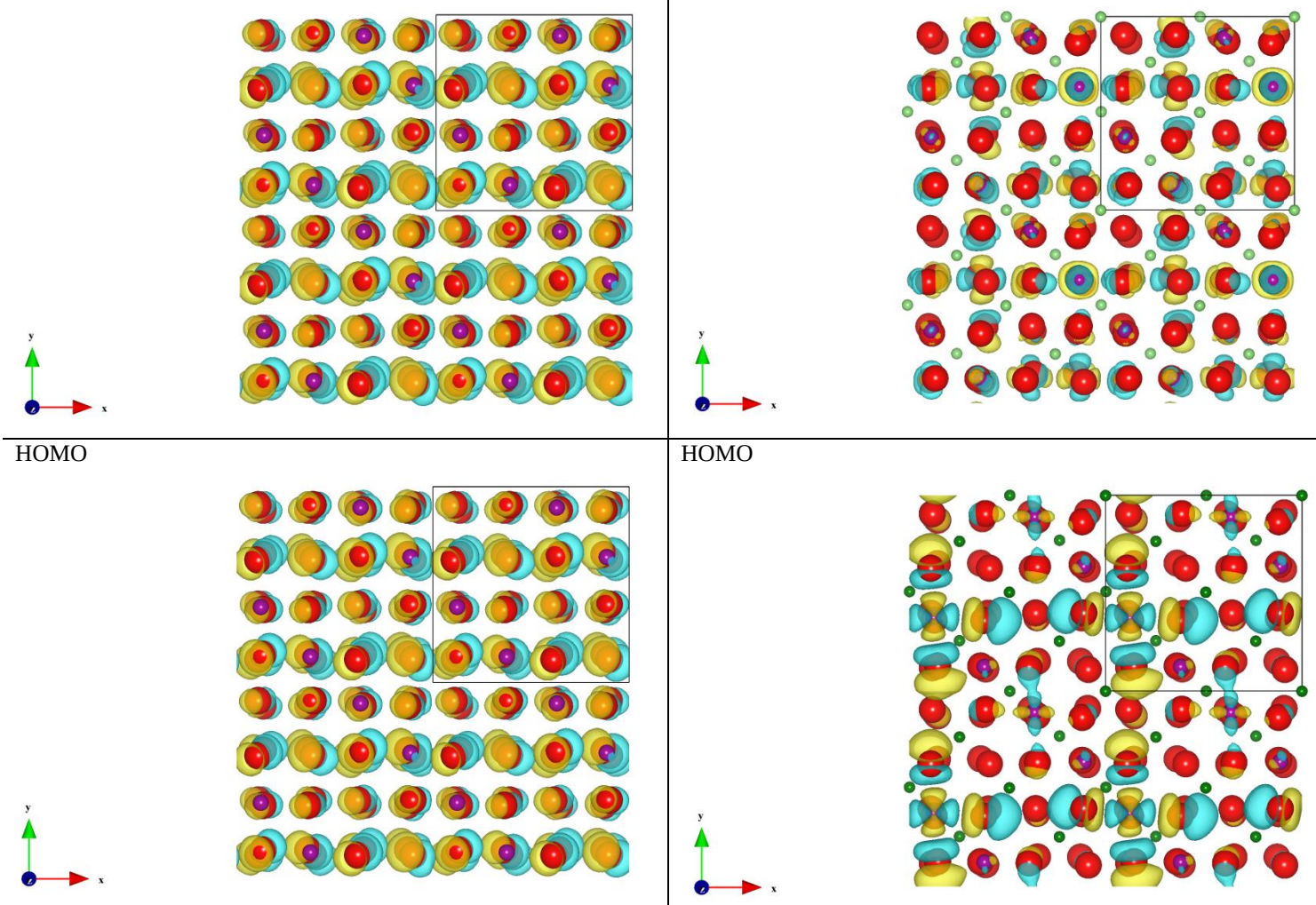

Figure S9. Representation of the frontier orbitals: HOMO and LUMO in optimized structure of $Mn_{16}O_{32}$ and $Li_8Mn_{16}O_{32}$ in (110) plane.

Electronic microscopy

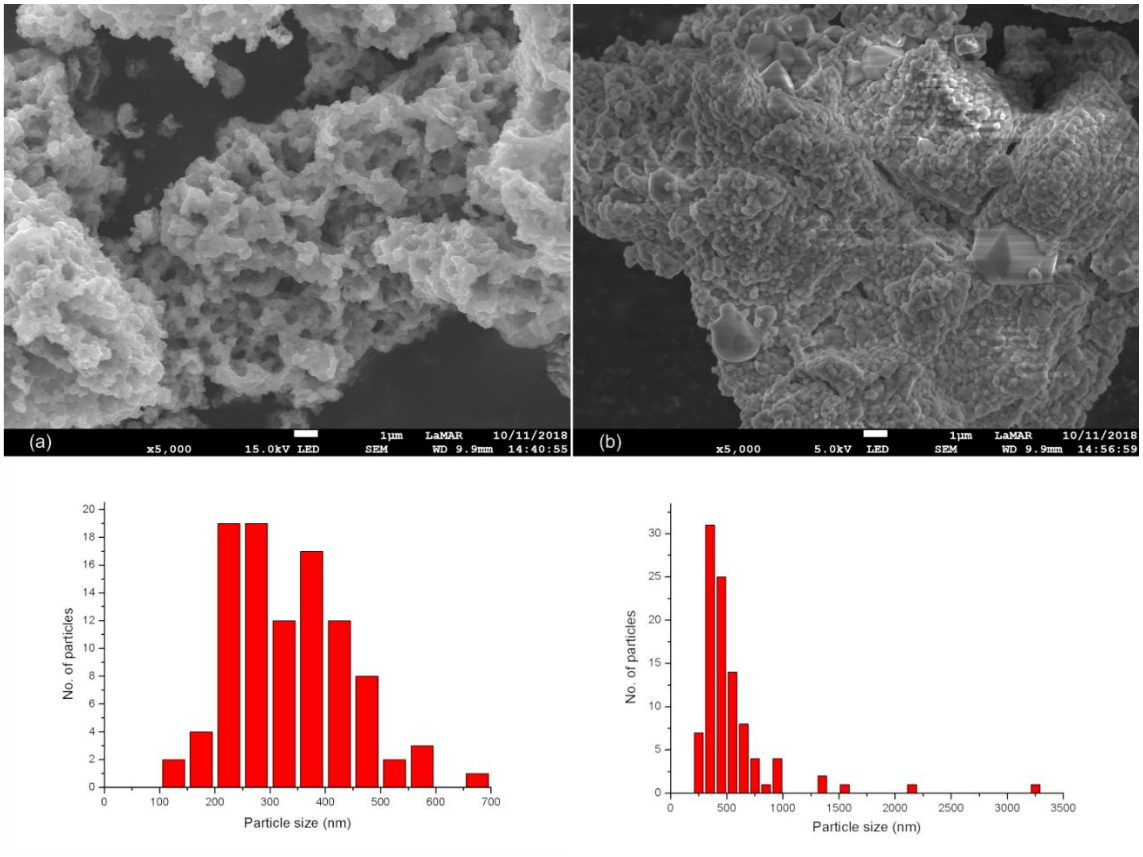

Figure S10. SEM images and histograms of $LiMn_2O_4$ treated at: (a) 500 and (b) 700 °C.

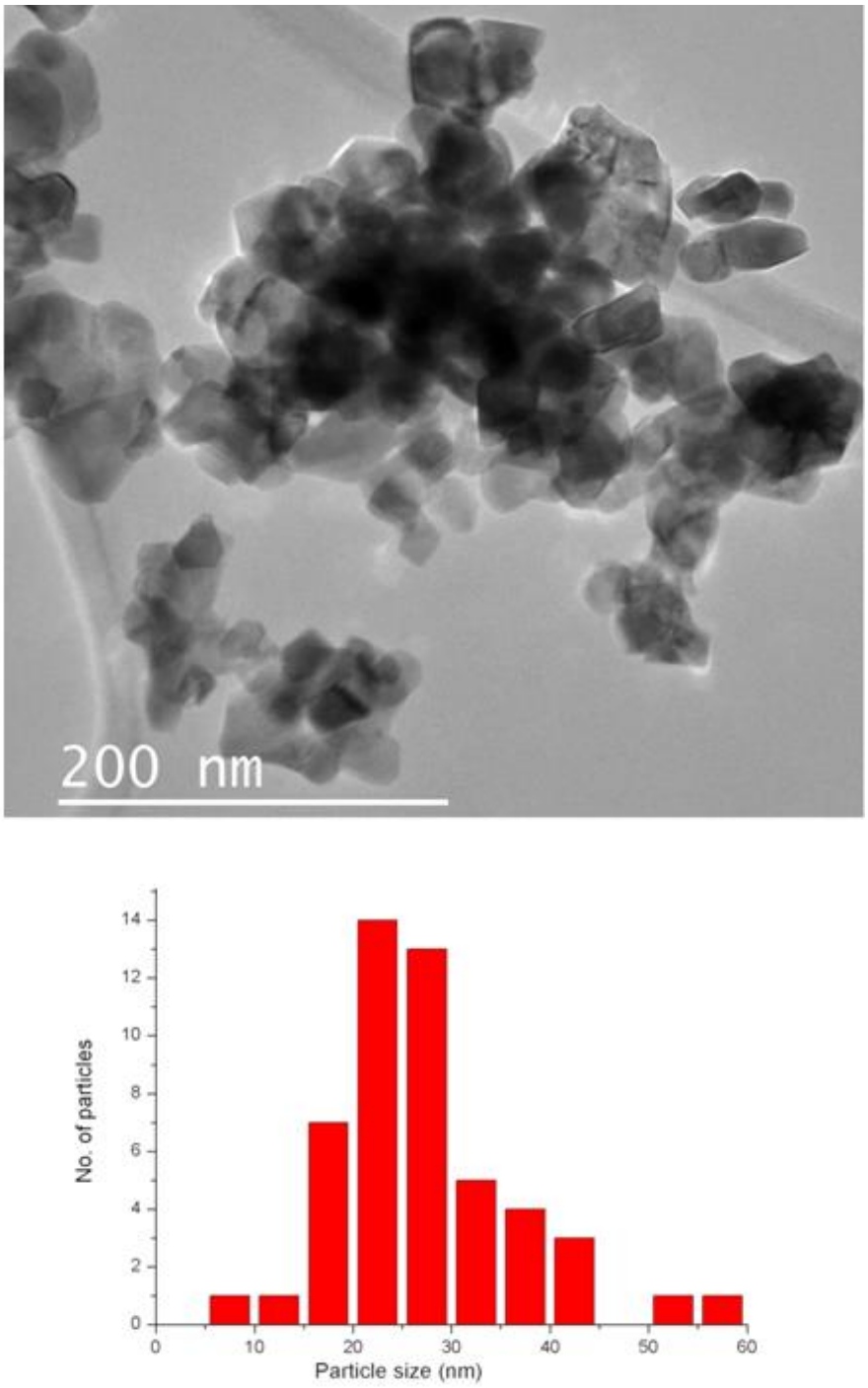

Figure S11. TEM image and histogram of $LiMn_2O_4$ treated at 700 °C.

References

1. Maniammal, K.; Madhu, G.; Biju, V.; *Phys. E* **2017**, *85*, 214.
2. Balzar, D. In *Defect and Microstructure Analysis by Diffraction*; IUCr/Oxford University Press: New York, 1999, p. 94.