Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Optimization effect of Ag-regulated manganese oxides on electrocatalytic performance for Li-O_2 batteries

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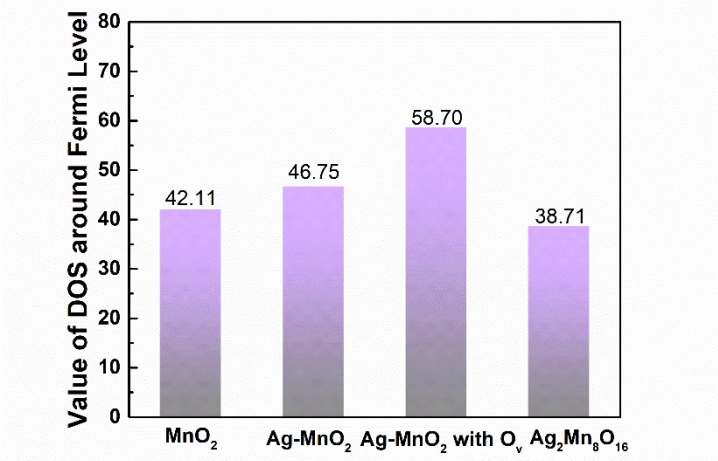

Figure S1. The values of DOS around Fermi level.

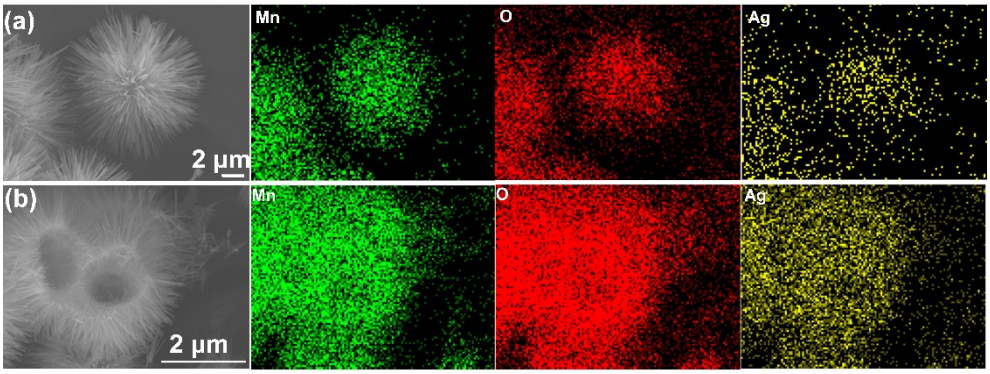

Figure S2. SEM image and corresponding EDS elemental mapping results of (a) Ag-MnO_2, (b) $Ag_2Mn_8O_{16}$.

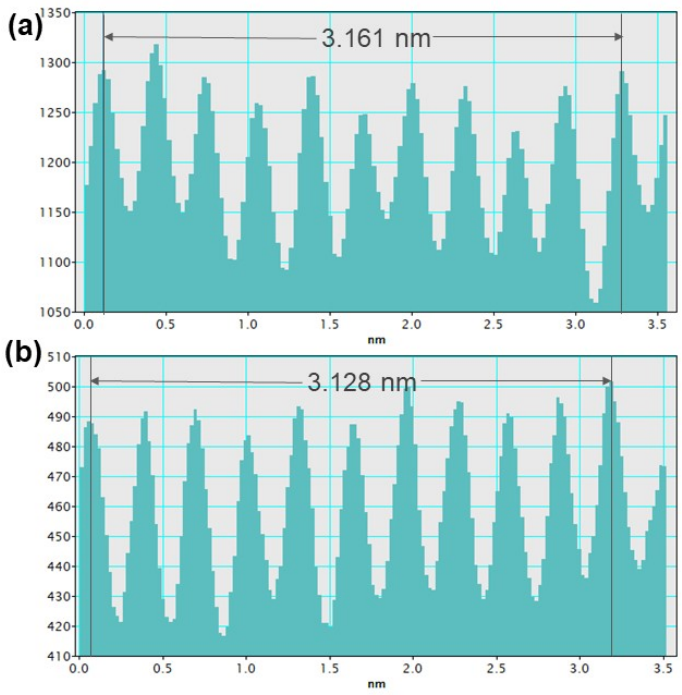

Figure S3. Profile of lattice fringes of (a) Ag-MnO_2 and (b) $Ag_2Mn_8O_{16}$.

Table S1. The adsorption energies (ΔE_{ads}) of LiO_2 and corresponding bonding parameters of (100) lattice plane.

Crystal	**d_{Li-O}（Å）**	**d_{Mn-O}（Å）**	**ΔE_{ads}（eV）**
α-MnO_2	1.938	1.947	-3.50
Ag-doped α-MnO_2	1.869	1.960	-2.30
Ag-doped α-MnO_2 with oxygen vacancy	1.851	1.948	-2.82

Table S2. Calculated cell parameters for MnO_2, Ag-MnO_2 and $Ag_2Mn_8O_{16}$.

Chemical composition		**MnO_2n**	**Ag-MnO_2**	**$Ag_2Mn_8O_{16}$**
Unit cell	*a* (Å)	9.878	9.806	9.780
Unit cell	*b* (Å)	9.878	9.806	9.780
Unit cell	*c* (Å)	2.859	2.848	2.861
Space group		*I4/m*	*I4/m*	*I4/m*
Calculated crystallite size ($Å^3$)		278.999	273.883	273.660
R_{wp}		3.89%	3.58%	2.74%
R_p		2.68%	2.64%	2.06%