PCCP

Electronic Supplementary Information

High temperature ferroelectric behaviour in α-MnO_2 nanorods realised through enriched oxygen vacancy induced non-stoichiometry

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1. HRTEM images confirming lateral aggregation

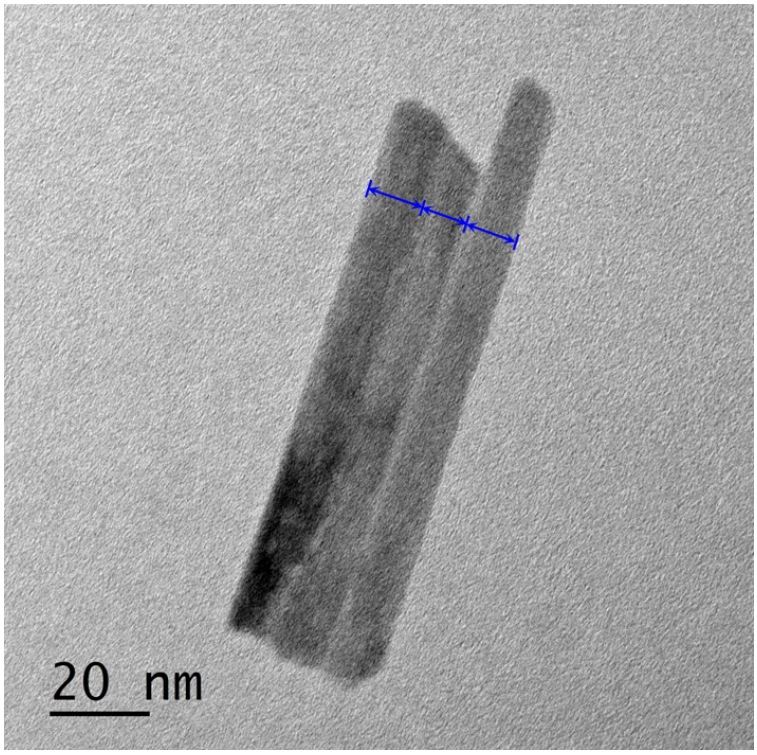

Fig. S1 HRTEM images of sample S1 depicting growth of nanorods through lateral aggregation

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2. $(MnO_2)_{surface} + H^+ + e^{-1} \longrightarrow MnOOH$

In the above equation the source of electron can be understood from the following reactions.

$ClO_3^- + 6H^+ \longrightarrow Cl^-(aq) + 3H_2O$ (1)

$2Cl^-(aq) \longrightarrow Cl_2(g) + 2e^{-1}$ (2)

The chlorine gas evolved during the reaction produces dense white fumes in presence of liquor ammonia. The thick white fumed are of ammonium chloride.

3. Calculation of dipole moment.

Displacement of the octahedral site cation from the geometric centre (x_0, y_0, z_0) can be obtained from equation (3)[1,2,3].

$$d = \sqrt{(x_0 - x)^2 + (y_0 - y)^2 + (z_0 - z)^2} \quad (3)$$

For the MnO_6 octahedron:

$$Dipole\ moment = d \times 4 \times 1.6 \times 10^{-19} \times 10^{-10}\ C\ m \quad (4)$$

Reference

[1] G. Lv, X. Xing, L. Wu, W. Jiang, Z. Li and L. Liao, *Sci. Rep.,* 2016, 6,37400.
[2] X. Wang, L. Mei, X. Xing, L. Liao, G. Lv, Z. Li and L. Wu, *Appl. Catal. B*, 2014, 160, 211.
[3] X. Xing, G. Lv, W. Xu, L. Liao, W.-T. Jiang, Z. Li and G.-S. Wang, *RSC Adv.*, 2016, 6, 58844.

