Supplementary Information for

"Observation of Ferroelectricity and Structure-Dependent Magnetic Behavior in Novel One-Dimensional Motifs of Pure, Crystalline Yttrium Manganese Oxides"

Jonathan M. Patete,[1] Jinkyu Han,[2] Amanda L. Tiano,[1] Haiqing Liu,[1] Myung-Geun Han,[2] J. W. Simonson,[3] Yuanyuan Li,[4] Alexander C. Santulli,[1] M.C. Aronson,[2,3] Anatoly I. Frenkel,[4] Yimei Zhu,[2] and Stanislaus S. Wong[1,2,*]

[1]Department of Chemistry, State University of New York at Stony Brook, Stony Brook, New York 11794-3400, USA

[2]Condensed Matter Physics and Materials Science Department, Building 480, Brookhaven National Laboratory, Upton, New York 11973, USA

[3]Department of Physics and Astronomy, State University of New York at Stony Brook, Stony Brook, New York 11794-3800, USA

[4]Department of Physics, Yeshiva University, New York, NY 10016

[*]Email: sswong@bnl.gov, stanislaus.wong@stonybrook.edu

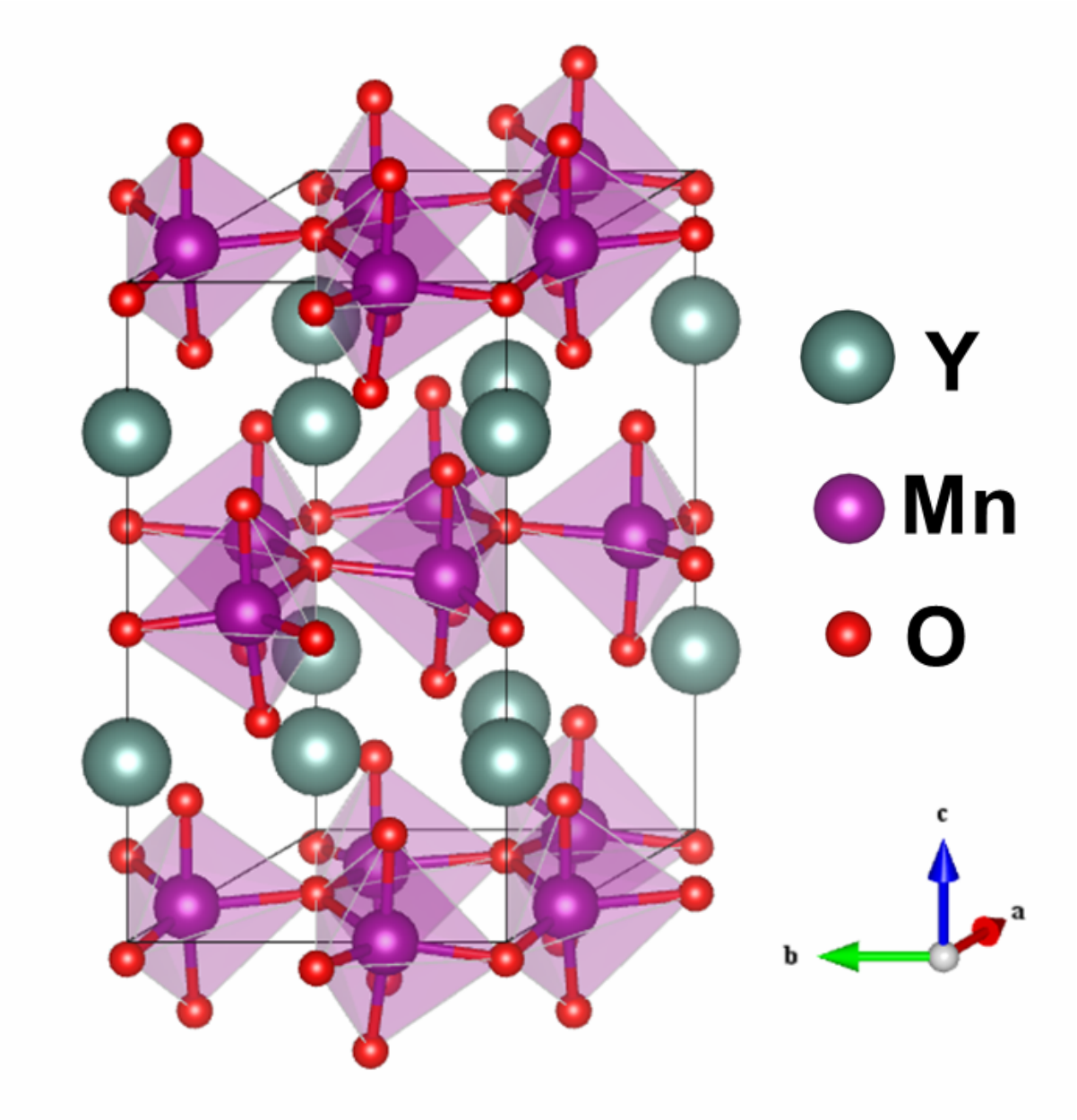

Figure S1. Unit cell representation of the crystal structure of hexagonal $YMnO_3$ (space group: P63cm). Green-blue, purple, and red spheres represent Y, Mn, and O ions, respectively. The polyhedral geometry of MnO_5 is depicted by the presence of purple shading.

XAFS analysis of $YMnO_3$: nanotubes, nanowires and 'bulk'

Raw data

Raw XAFS data (Figure S2) are shown in energy, k-space and r-space. It is evident that the nanotubes have identical local geometry and electronic structure with the bulk. Nanowires have somewhat different local structure as evidenced by the changes in the XANES and EXAFS regions. The nature of the change can be either due to the different coordination numbers of Y-Y, Y-Mn and Mn-Mn contributions to the second peak in r-space, or to standard deviations in their bond lengths, or both. In our analysis scheme, we have assumed that the structural framework remains the same; only the distances and their disorder parameters change between different compounds. That model was incorporated in the theoretical calculation, done using FEFF6.

Table S1. Mean square disorder (in $Å^2$) in the interatomic distances between the nearest neighbors to Mn and Y as obtained by EXAFS analysis in the three measured materials: nanotubes, nanowires, and bulk.

System	**Mn-O**	**Mn-Y1**	**Mn-Mn**	**Mn-Y2**	**Y-O**	**Y-Mn1**	**Y-Y**	**Y-Mn2**
Bulk	0.0103 ± 0.0022	0.0064 ± 0.0012	0.0220 ± 0.0061	0.0064 ± 0.0012	0.0057 ± 0.0015	0.0064 ± 0.0012	0.0053 ± 0.0012	0.0064 ± 0.0012
NW	0.0094 ± 0.0014	0.0121 ± 0.0030	0.0219 ± 0.0086	0.0121 ± 0.0030	0.0080 ± 0.0014	0.0121 ± 0.0030	0.0055 ± 0.0011	0.0121 ± 0.0030
NT	0.0104 ± 0.0011	0.0069 ±0.0013	0.0210 ± 0.0053	0.0069 ± 0.0013	0.0059 ± 0.0020	0.0069 ± 0.0013	0.0054 ± 0.0017	0.0069 ± 0.0013

Mn *K*-edge and Y *K*-edge data

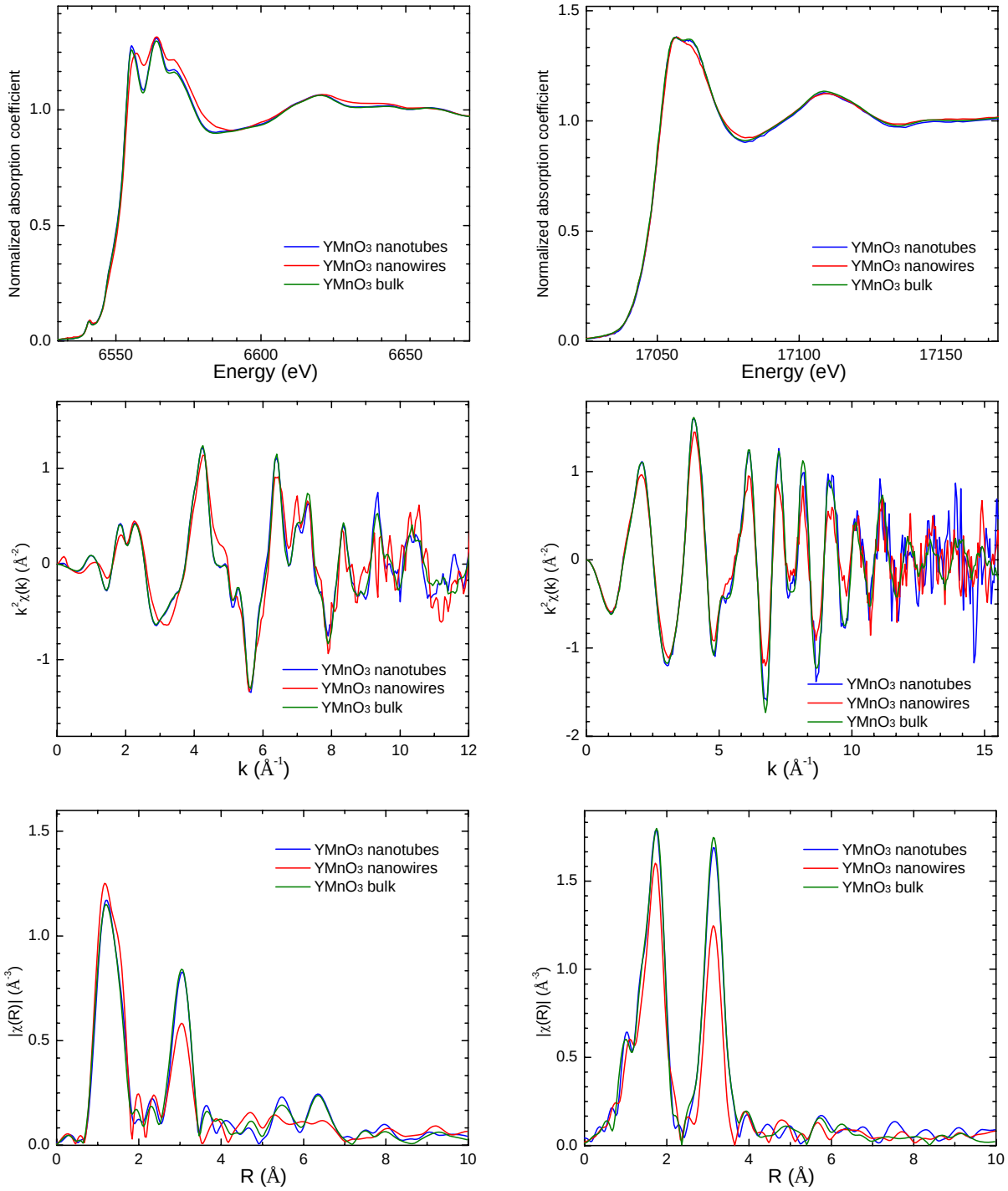

Figure S2. Raw data in energy, *k*-space, and *r*-space for the M *K*-edge (left) and Y *K*-edge (right) for $YMnO_3$ nanotubes, nanowires, and for the bulk samples. Both the Mn and Y edge data indicate that the local structure of the nanotubes is identical to the bulk, whereas the structure of nanowires is slightly different. The nature of the difference is likely to be larger structural disorder in the Mn and/or Y sites in the nanowires as compared with the nanotubes and the bulk.

Mn K-edge and Y K-edge

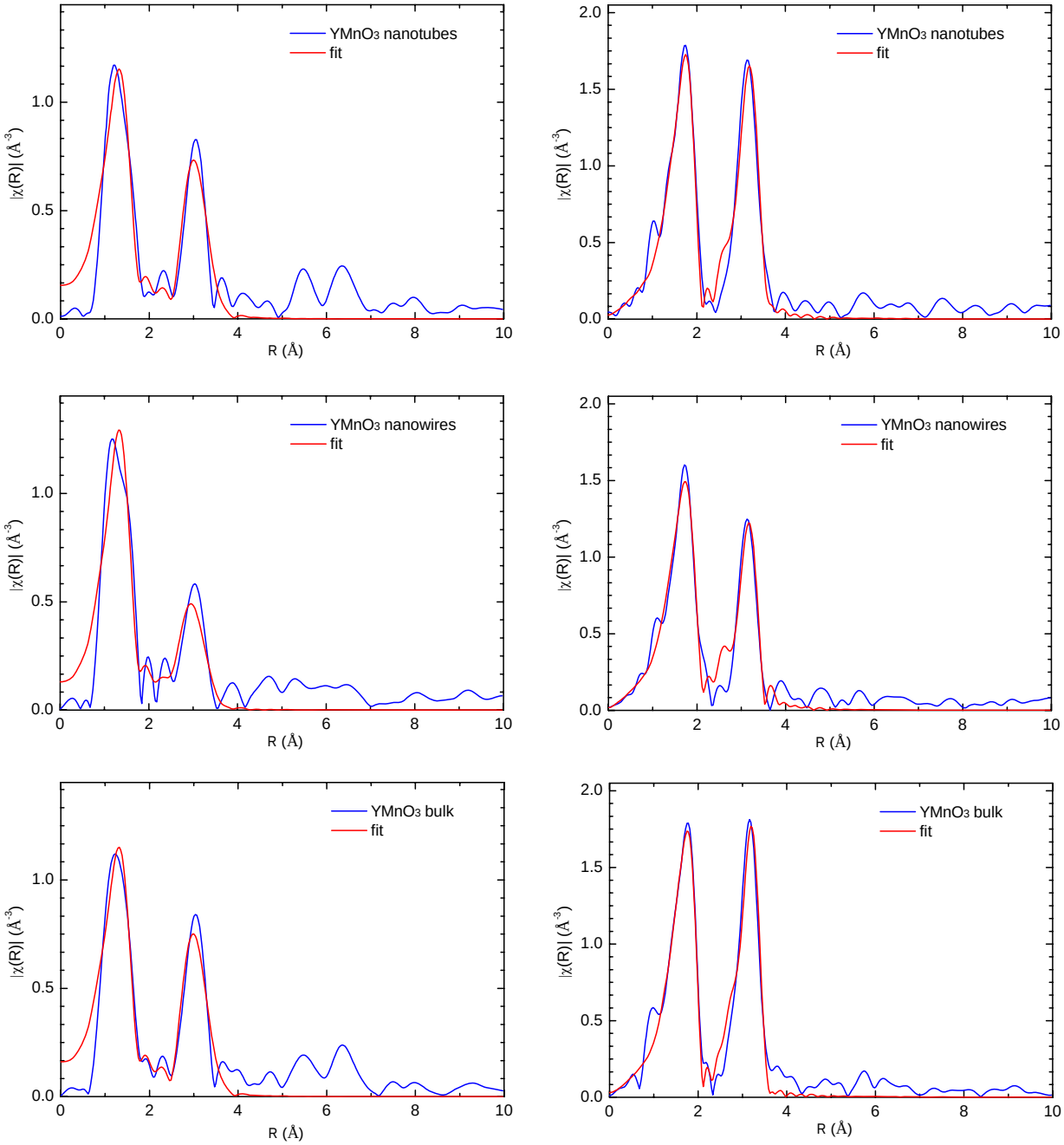

Figure S3. Fourier transform of k^2-weighted EXAFS data and theoretical fits to the M *K*-edge (left) and Y *K*-edge (right) for $YMnO_3$ nanotubes, nanowires, and bulk samples.

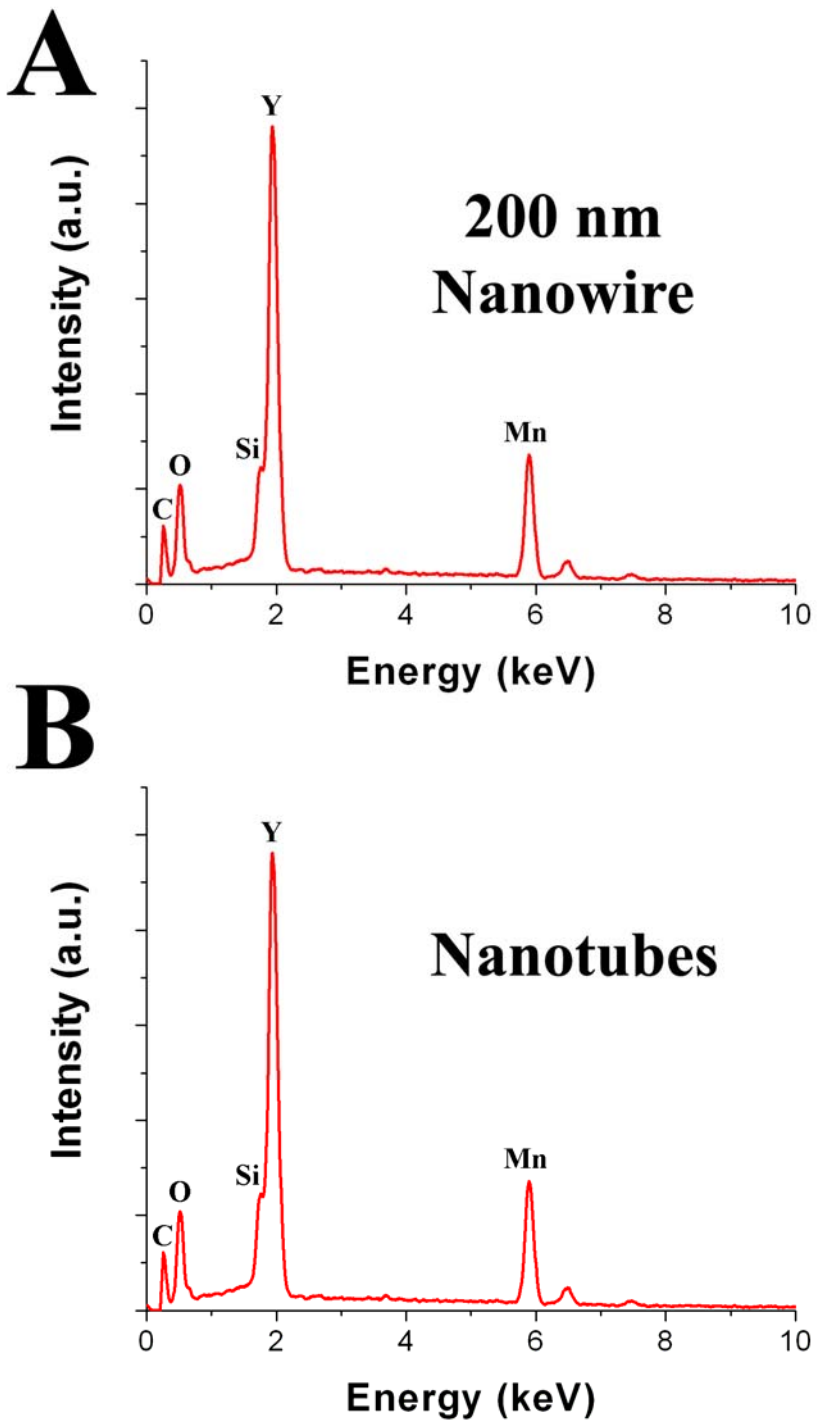

Figure S4. Energy dispersive X-ray spectra of as-prepared sol-gel synthesized nanowires (A) and nanotubes (B).

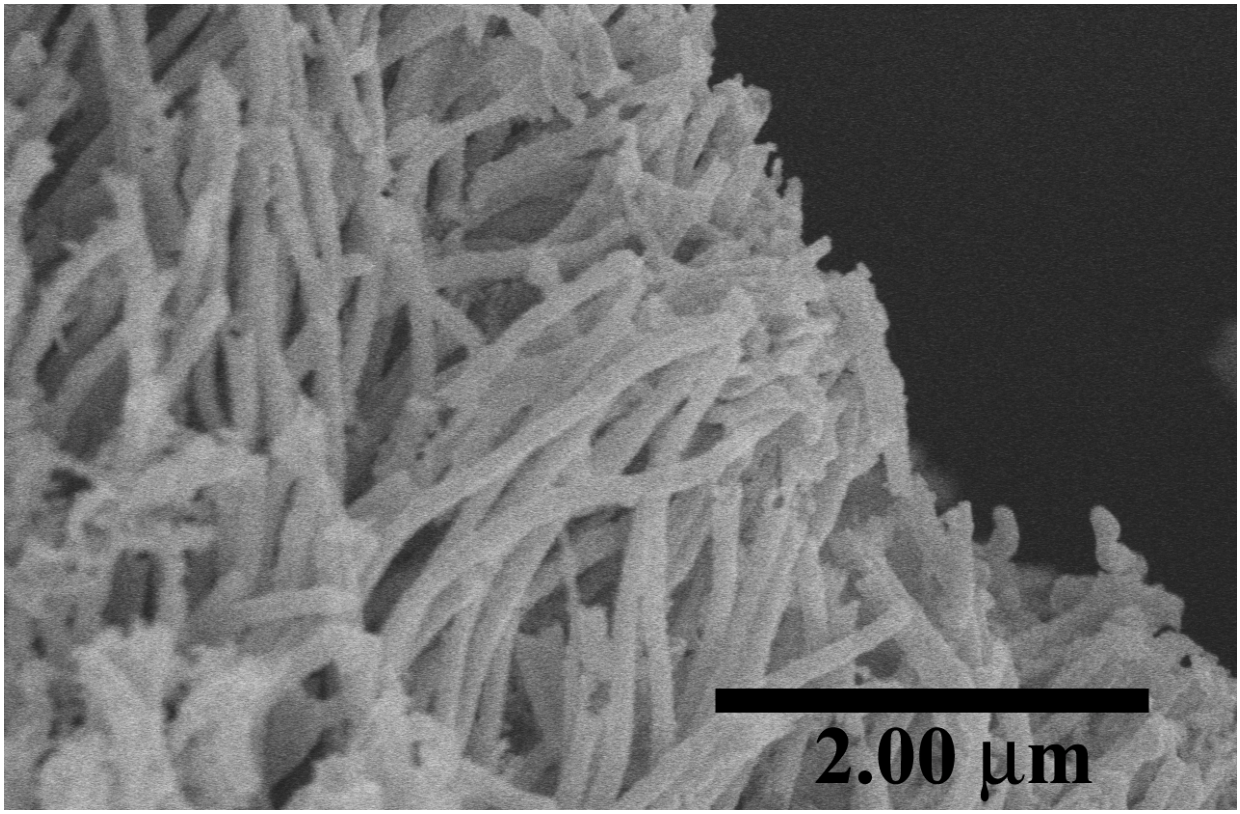

Figure S5. SEM image of representative nanowire bundles obtained from annealing the amorphous product within the template.

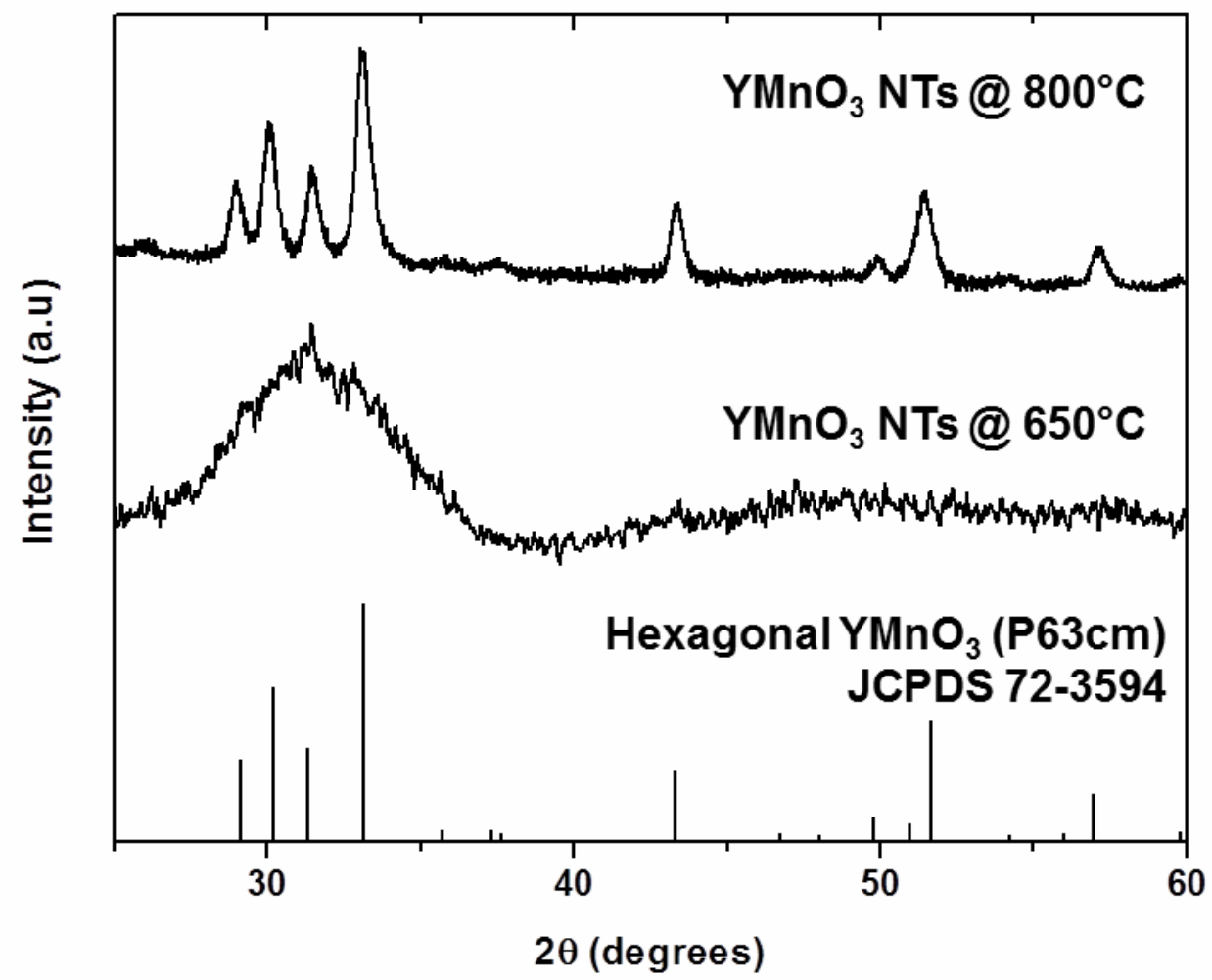

Figure S6. X-ray diffraction patterns for $YMnO_3$ nanotubes calcined at 650°C (bottom) and annealed at 800°C (top). The black lines correspond to the Bragg peak positions of the bulk $YMnO_3$ which can be described by JCPDS #72-3594.

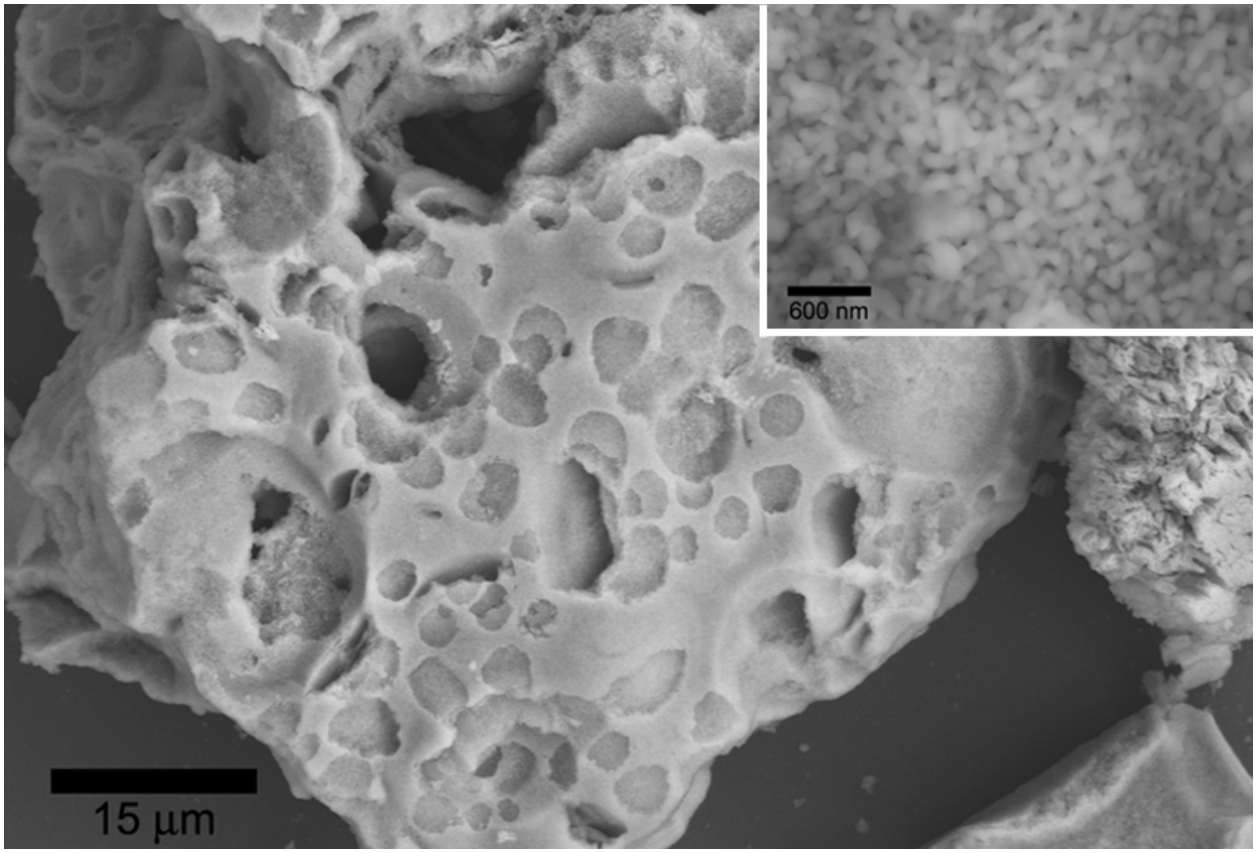

Figure S7. A representative SEM image (with a higher resolution inset) of the *h*-$YMnO_3$ product obtained from annealing the precursor sol in a porcelain coated boat, without the use of a template. This sample highlights the "bulk" control sample.