Supporting Information for:

**Insights into the capping and structure of MoS$_2$ nanotubes as revealed by aberration-corrected STEM**

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**MoO$_3$ nanobelts**

In a typical synthesis, 100 mg of Mo powder was placed in a 250 mL beaker in a Petri dish with water on a magnetic stirring plate. Under light stirring, 10 mL of H$_2$O$_2$ (30 wt % in H$_2$O) was then added slowly. The solution rapidly turned to an orange-yellow color. After 10 minutes of continuous stirring, the clear orange solution was transferred to a Teflon container which was then loaded into an autoclave. The autoclave was heated in an oven at 180 °C for 12-24 hours. After this time period, the autoclave was allowed to cool and the white powder was collected and washed thrice with H$_2$O and ethanol and dried overnight in the oven.

Figs. 1a and b show the SEM and TEM images of the MoO$_3$ nanobelts synthesized using Mo powder and H$_2$O$_2$. Large yields of the as-synthesized nanobelts can be clearly seen from the images. The length of the nanobelts extends up to several tens of microns whereas the diameter of the nanobelts is in the 300-500 nm range (Fig. S1b). The selected area electron diffraction (SAED) pattern shown in Fig. S1c reveals the single crystal structure of the nanobelts with diffraction spots corresponding to (002) and (200) lattice planes of orthorhombic MoO$_3$ (α-MoO$_3$). The nanobelts grow along the <001> direction due to the intrinsic structural anisotropy and growth rate ($r_{hkl}$) variation in all three principal directions $r_{001} > r_{100} > r_{010}$.$^{1,2}$ The SEM-EDAX spectrum (Fig. S1d) confirms the presence of the respective elements of Mo and O as revealed by the characteristic and distinct Mo (K,L) and O (K) lines. The atomic ratio of Mo:O is found to be close to 1:3. Further evidence for the presence of only Mo and O in the nanobelts can be inferred from the elemental maps of Mo (Mo-L) and O (O-K) (Fig. S1e and f).

**MoS$_2$ nanotubes**
Fig. S2 shows the SEM image of the MoS$_2$ nanotubes that were obtained starting from the MoO$_3$ nanobelts and using a mixture of gases of H$_2$/H$_2$S at 900 °C. Copious amounts of nanotubes were obtained during the synthesis as can be seen from the images wherein the length of the nanotubes extends upto a micron.

Fig. S3a depicts the HRTEM images of well faceted MoS$_2$ nanotubes. The nanotube of ~100 nm in diameter exhibits an unusual faceted closed end. The thickness of the wall is approximately 15 nm and the nanotubes have about 15-20 layers (Fig. S3b). The individual and distinct layers are clearly differentiated in the image. The layers correspond to the d$_{002}$ planes, with a lattice distance of 0.633 nm, as shown by the line profile in Fig. S3c. STEM-HAADF images of the MoS$_2$ nanotubes, obtained from a JEOL 2100F operated at 200 kV, with a probe size of 0.5 nm, are shown in Fig. S3d. A close-up view of the individual layers of the nanotubes is shown in Fig. S3e (corresponding to the region marked by the box in Fig. S3d). The fact that the nanotubes are composed of only Mo and S is revealed by the line scan analysis that was carried out along the entire diameter of the nanotube (Fig. S3f). The compositional analysis revealed a ratio of 1:2 between Mo and S, in accordance to the formation of MoS$_2$.

A schematic representation of the various cap formations are shown in Fig. S4. Fig. S4a shows the schematic of the sharp 90° bends of the cap with respect to the nanotube. The two variations in the conical capped nanotubes are shown in the schematics in Figs. 4b and 4c. The more faceted octagon-like capped structure is shown in the schematic of Fig. S4d.

**Figure Captions**

**Fig. S1**
(a) and (b) SEM and TEM images of the MoO$_3$ nanobelts synthesized from Mo powder and H$_2$O$_2$, (c) SAED pattern of α-MoO$_3$ taken along the [010] orientation of the crystal and indexed assuming orthorombic symmetry, (d) EDAX spectrum of the MoO$_3$ nanobelts and the corresponding elemental maps of Mo (L) (e) and O (K) (f).

**Fig. S2**
(a) and (b) SEM image of the MoS$_2$ nanotubes that were obtained starting from the MoO$_3$ nanobelts and using a mixture of gases of H$_2$/H$_2$S at 900 °C.
Fig. S3  (a) TEM image of a MoS$_2$ nanotube with an unusual faceted closed cap, (b) Closer look at the capped end of the nanotubes: HRTEM image of the capped edge of the MoS$_2$ nanotube showing the lattice fringes corresponding to the d$_{002}$ layers, (c) Line profile showing the spacing of the MoS$_2$ layers to be 0.63 nm, (d) STEM-HAADF image of a MoS$_2$ nanotube, (e) A High resolution STEM image of one of the corners, marked by a square, is shown, f) A line scan analysis carried out on the nanotube shows the composition of Mo (in blue) and S (red).

Fig. S4  (a)–(d) Schematic models showing the different caps observed in the present study, (a) Nanotube with a flat cap structure, (b) and (c) Variations of the conical caps, (d) Nanotube with a half-octagon cap.

References
Fig. S1
Fig. S2
Fig. S3

Fig. S4