Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Rapid augmentation of vertically aligned MoO_3 nanorods *via* microwave irradiation

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1. Materials and Methods

Ammonium heptamolybdate tetrahydrate, AHM (99.9 %) and concentrated nitric acid (69%) were purchased from Merck. All other reagents were of analytical grade and used without further purification. All aqueous solutions were prepared with Milli-Q water. Field emission scanning electron microscope (TESCAN MIRA 3 LM, Brno, Czech Republic) and attached Bruker Nano XFlash 6130 was used to study surface morphology of nanorods and perform energy dispersive spectroscopy (EDS). X-ray diffraction measurements were carried out using Rigaku Smart Lab diffractometer with Cu-Kα (40 kV, 30 mA) and Raman spectroscopy studies were carried out using Horiba XploRA PLUS spectrometer. FEI Tecnai (T20 S-TWIN TEM, 200kV) transmission electron microscope was used to perform the structural characterization of the h-MoO_3 nanorods. Absorption, transmission, and emission spectra were acquired using Perkin-Elmer Lambda 750 and Horiba Jobin-Yvon (Flourolog-3).

2. Supplementary Results

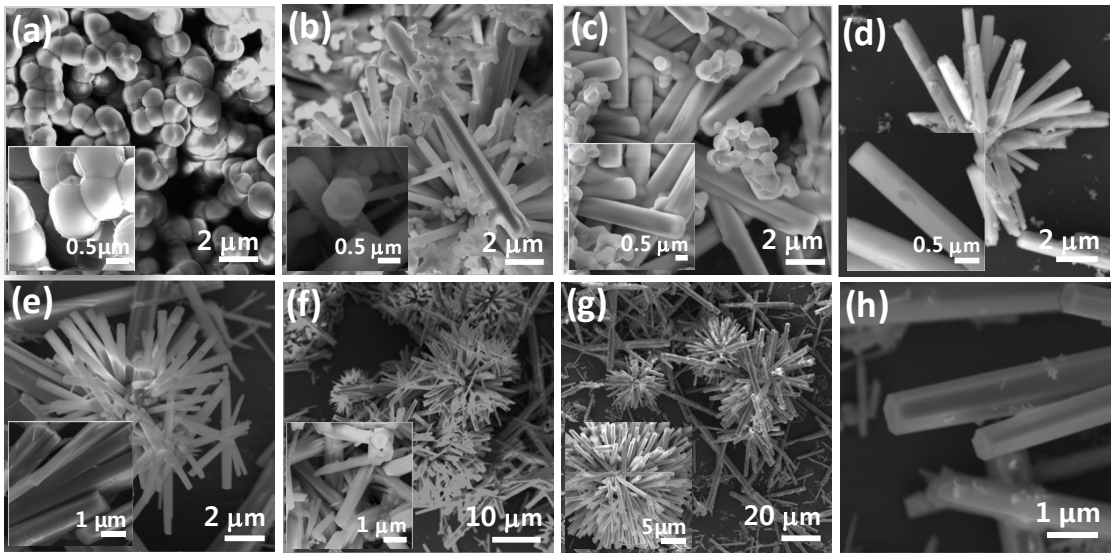

Figure S1. Microwave power dependant formation of h-MoO_3 NRs in solution phase with increase in power of (a) 80 (b) 160 (c) 240 (d) 320 W (e) 400 W (f) 480 W (g) and (h) 560 W and zoom-in view (inset) employing irradiation time of 300 s and AHM concentration of 0.02 M.

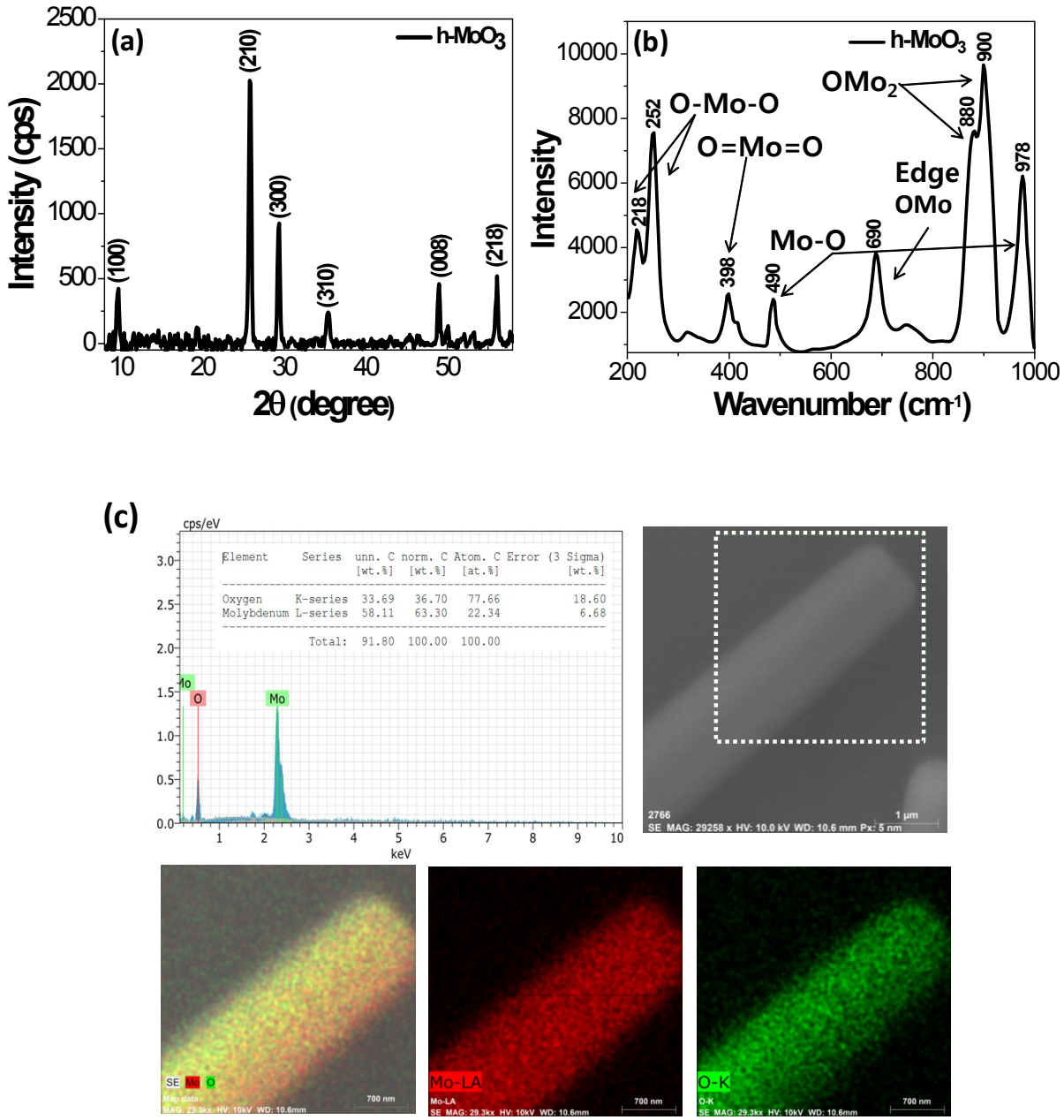

Figure S2. (a) XRD (b) Raman [1-3] and (c) EDS analysis of h-MoO_3 NRs synthesized in solution phase at 320W microwave power for 300 s of irradiation with AHM concentration of 0.02 M.

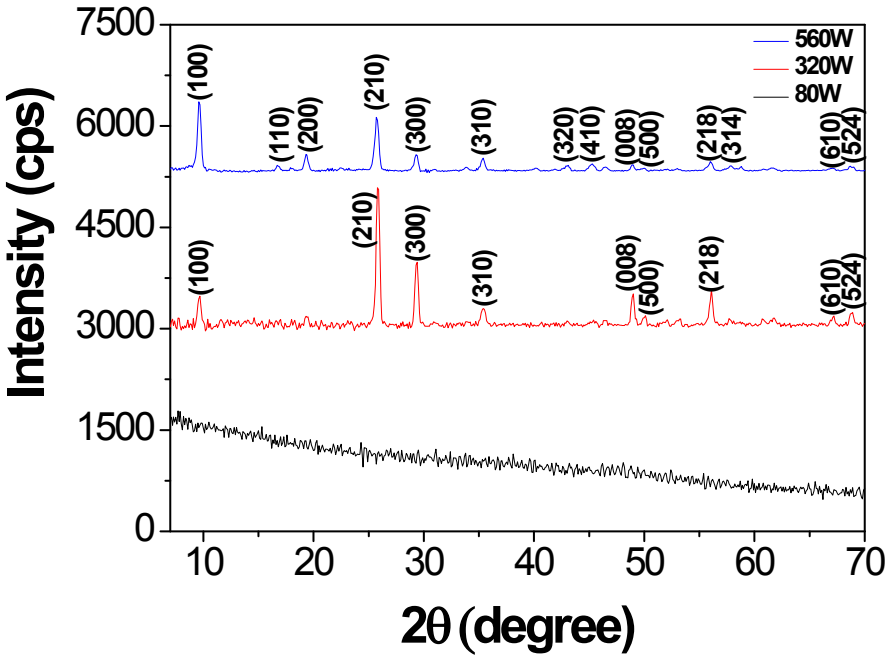

Figure S3. XRD pattern of the comparative study of microwave power dependency on h-MoO_3 NRs obtained in solution phase at 80, 320 and 560 W with 300 s of irradiation and AHM concentration of 0.02 M.

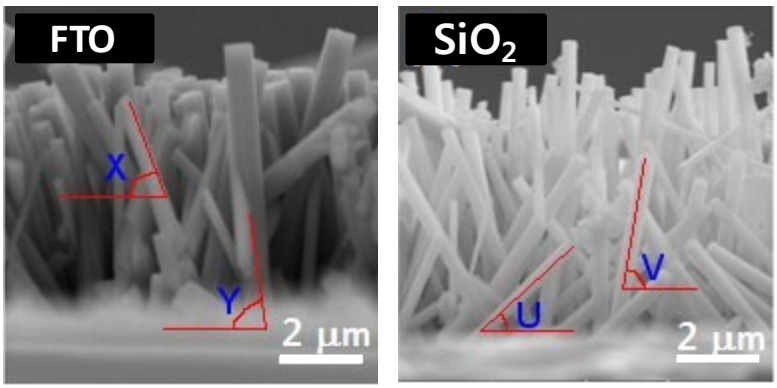

Figure S4. Calculation of inclination angle of vertically grown h-MoO_3 nanorods on FTO and SiO_2, where X= 70 deg ; Y=84 deg; U=42 deg; V= 81 deg (representative values of angle determination)

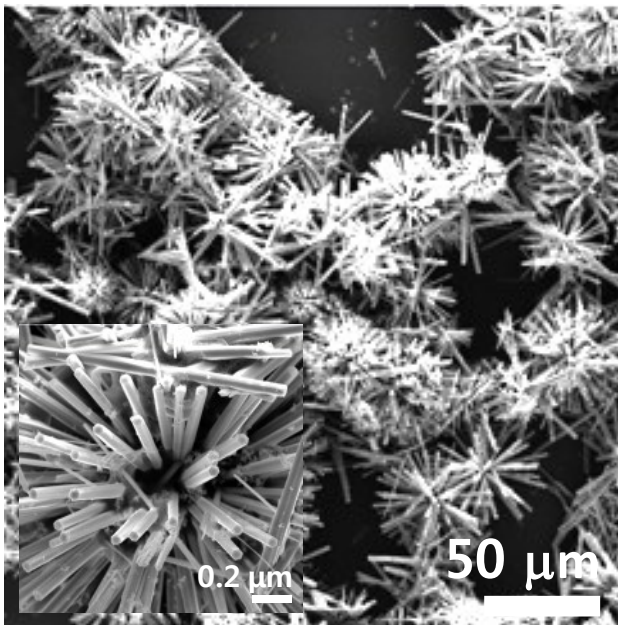

Figure S5. FESEM image of h-MoO_3 NRs grown on unseeded FTO substrate employing microwave irradiation time of 300 s, power of 320 W and AHM concentration of 0.02 M and zoom-in view (inset).

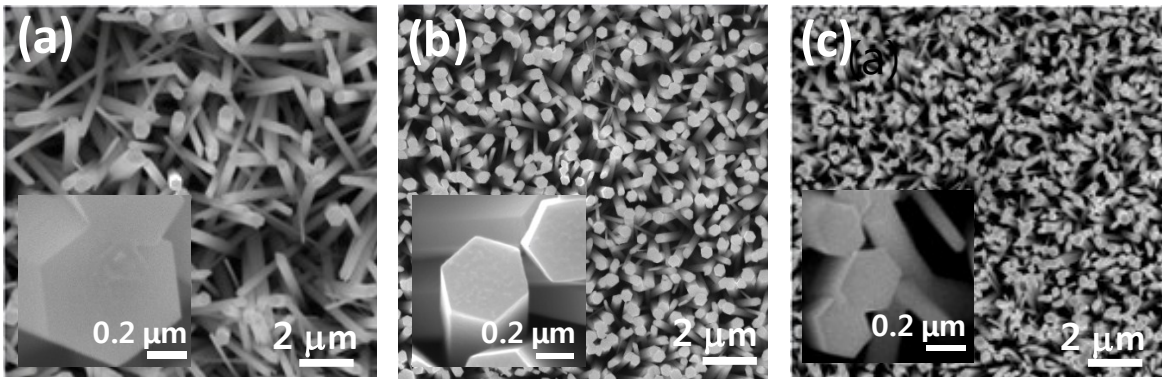

Figure S6. Concentration dependant vertical growth of h-MoO_3 NRs on FTO substrate obtained using microwave irradiation of 320 W and for 300 s. (a) 0.01 M (b) 0.02 M (c) 0.05 M and their zoom-in view (inset) showing top view.

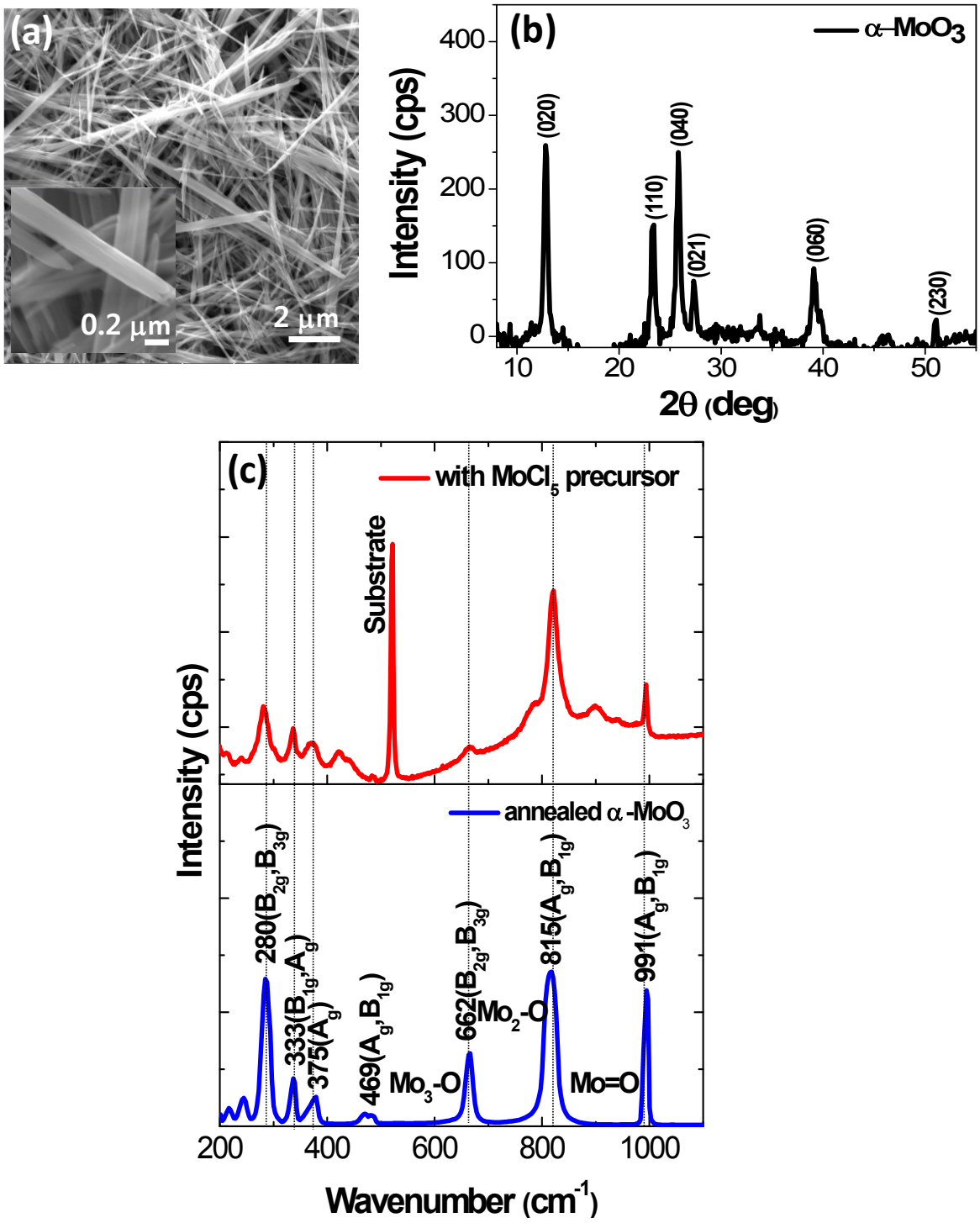

Figure S7. (a) FESEM, zoom-in view (inset) and (b) XRD analysis of α-MoO_3 NRs synthesized in solution phase using a different precursor; $MoCl_5$ employing a microwave power of 320 W and 300 s of irradiation time (c) Raman spectra of α-MoO_3 prepared by $MoCl_5$ precursor and annealing of h-MoO_3 nanorods.

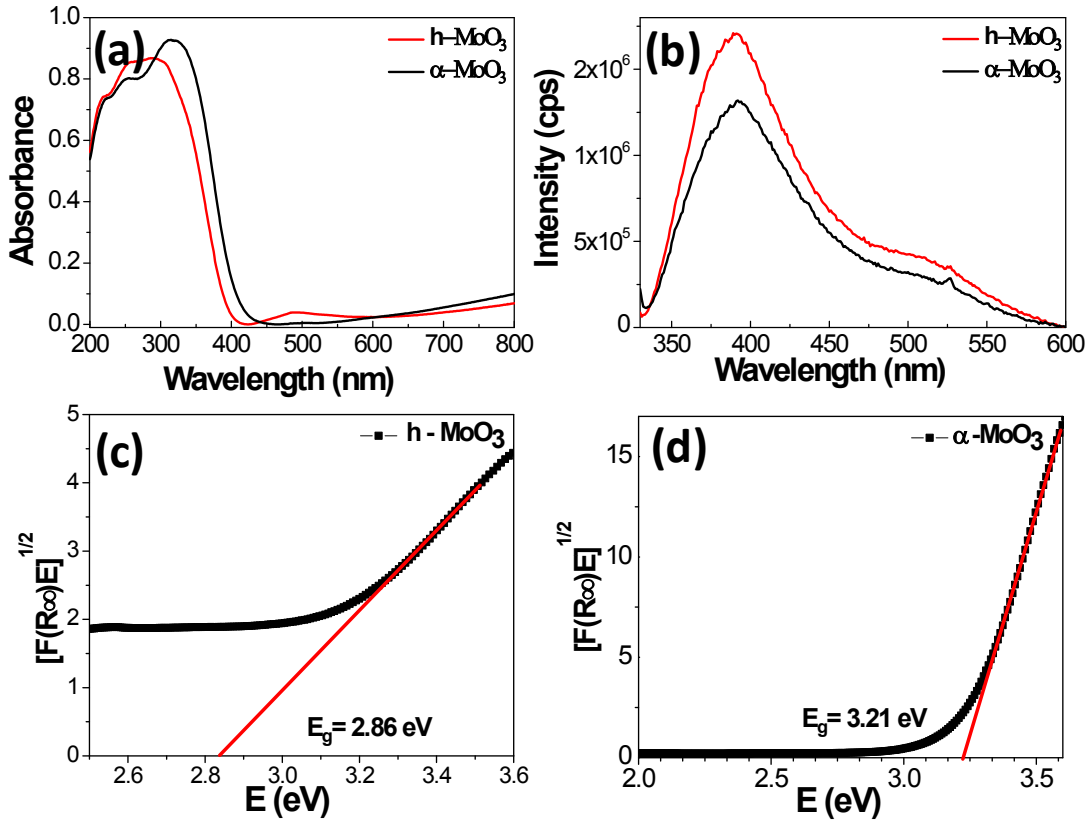

Figure S8. (a) and (b) absorption and photoluminescence spectra of h-MoO_3 and α-MoO_3 (c) and (d) optical band gap calculation

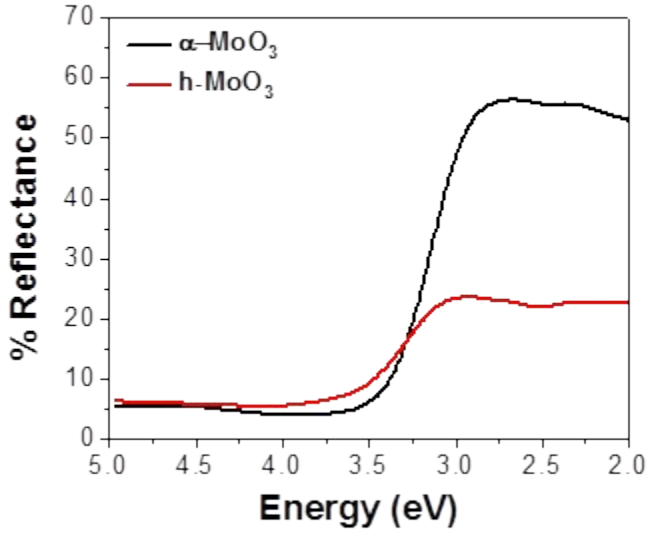

Figure S9. Diffuse reflectance spectra of vertically aligned h-MoO_3 NRs on FTO obtained by microwave synthesis and α-MoO_3 NRs obtained after annealing of the same.

Table S1. Average dimensions of vertically aligned h-MoO_3 NRs synthesized at various conditions (a) Microwave power (300 s, 0.02 M AHM; solution phase) (b) substrate (300 s, 320 W, 0.02 M AHM, vertical growth) and (c) AHM concentration (300 s, 320 W, FTO substrate, vertical growth).

(a) Microwave Power

Power (W)	Length (µm)	diameter (µm)	Aspect Ratio (µm)
160	4.5	0.4	11.3
320	5.7	0.62	9.2
560	54.2	2.6	20.8

(b) Substrate

Substrate	Length (µm)	diameter (µm)	Aspect Ratio (µm)
FTO	5.84	0.42	13.9
SiO_2	6.28	0.17	36.9

(c) AHM concentration

Concentration (M)	Length (µm)	diameter (µm)	Aspect Ratio (µm)
0.01	6.25	0.75	8.3
0.02	5.84	0.42	13.9
0.05	5.6	0.3	18.7

Table S2. Summary of solution based synthesis of h-MoO_3 nanorods

Power (W)	Morphology	Diameter (μm)
80	Spherical	0.9 - 1.1
160	Rod shaped and Spherical particles	0.3-0.5
240	Rod shaped with rounded edges	0.3-0.6
320	Rods with well defined hexagonal edges	0.4 - 0.7
400	Rods with well defined hexagonal edges	0.6 – 1.3
480	Broken hexagonal nanorods with defects	1.1 - 1.5
560	Broken hexagonal nanorods with defects	1.8 – 2.3

1. Notes and references

1. W. Pan, R. Tian, H. Jin, Y. Guo, L. Zhang, X. Wu, L. Zhang, Z. Han, G. Liu and J. Li, *Chemistry of Materials*, 2010, **22**, 6202-6208.
2. M. Camacho-López, E. Haro-Poniatowski, L. Lartundo-Rojas, J. Livage and C. Julien, *Materials Science and Engineering: B*, 2006, **135**, 88-94.
3. D. Liu, W. Lei, J. Hao, D. Liu, B. Liu, X. Wang, X. Chen, Q. Cui, G. Zou and J. Liu, *Journal of Applied Physics*, 2009, **105**, 023513.