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ARTICLE

Role of synthesis variables on controlled nucleation and growth of hexagonal molybdenum oxide nanocrystals: Investigation on thermal and optical properties

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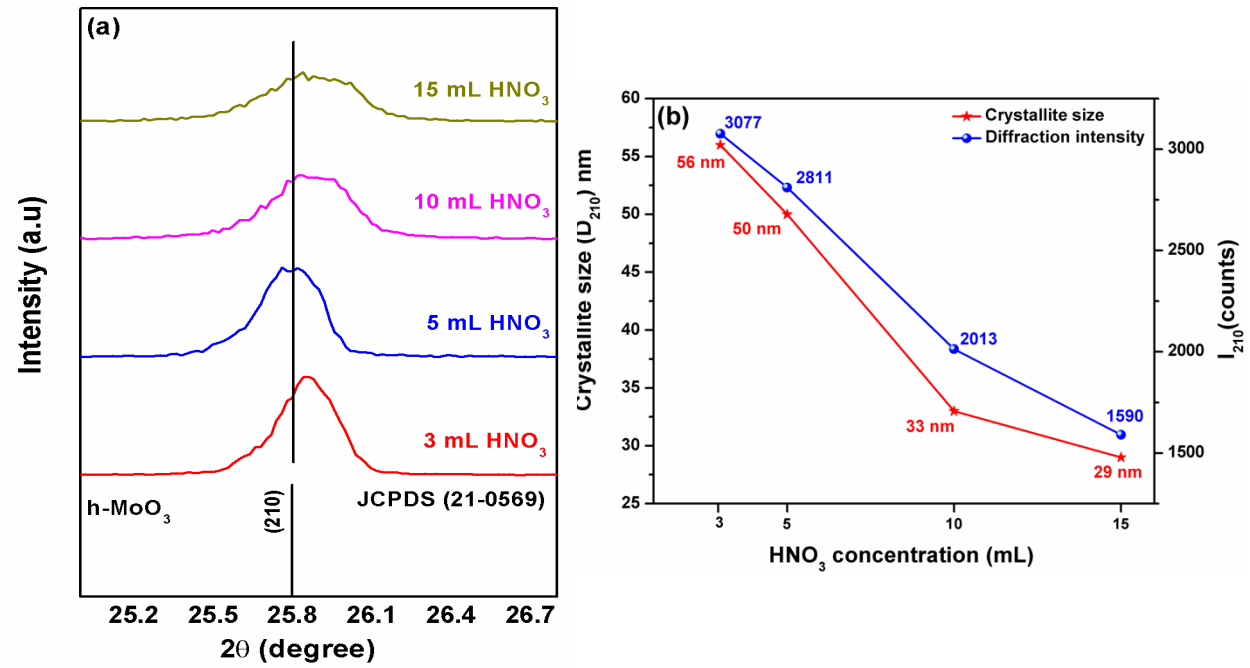
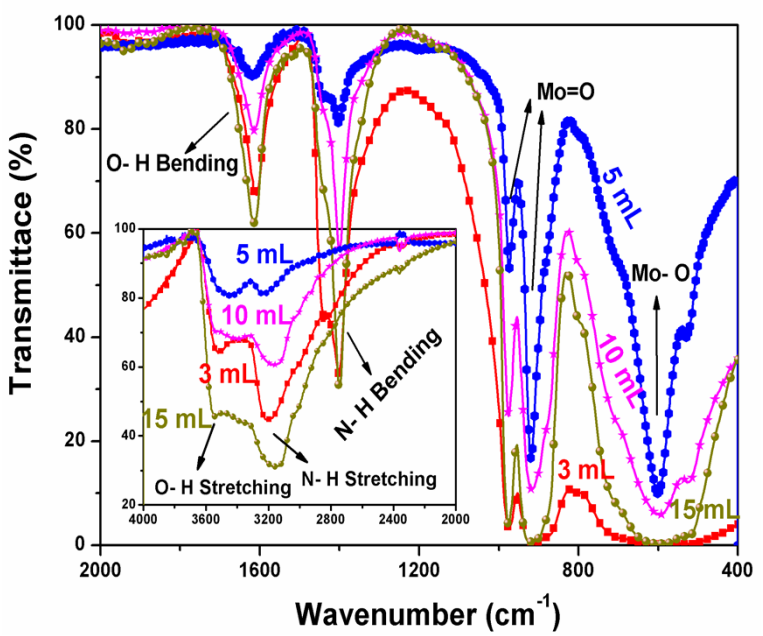
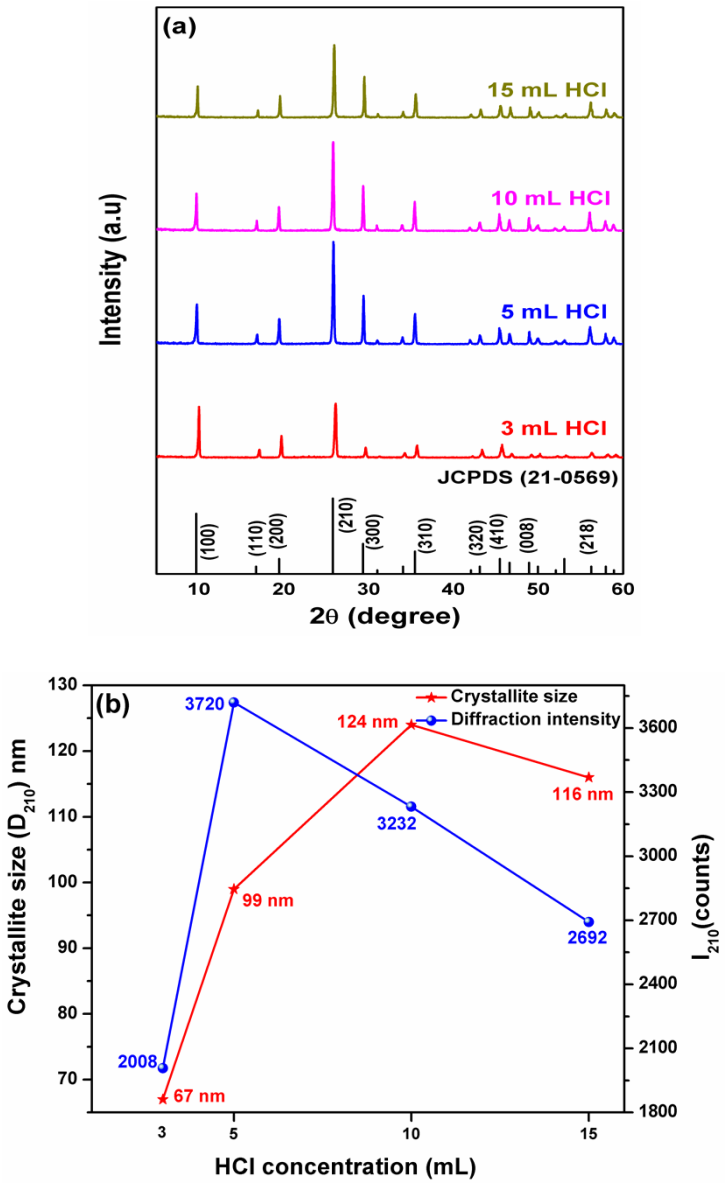


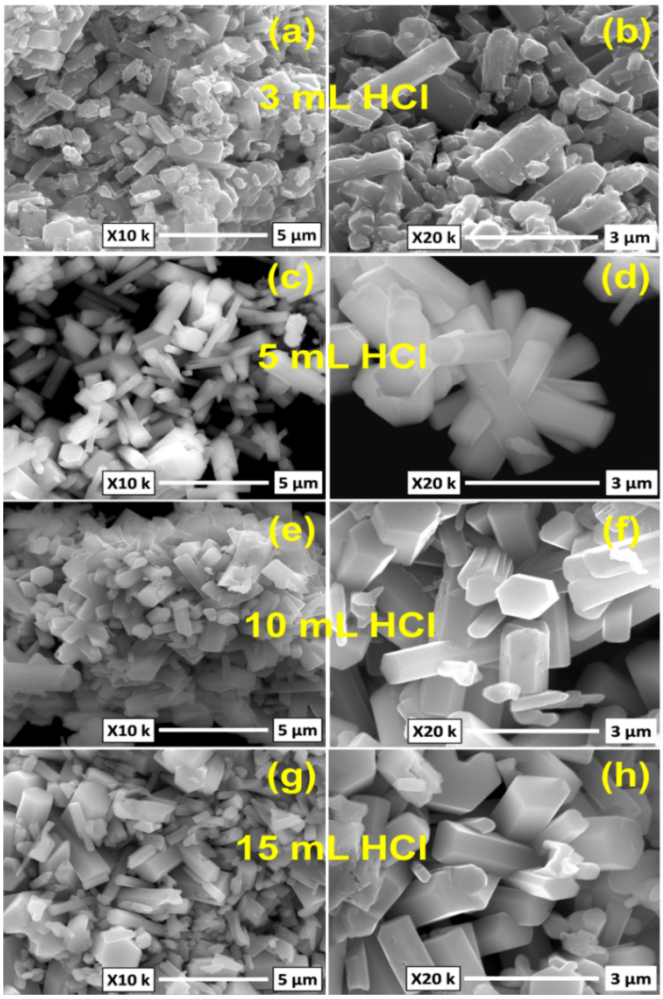
(ESI†) S1(a) The peak shift analysis of as-synthesized h-MoO_3 samples prepared with different HNO_3 concentrations; **(b)** variation of diffraction peak intensity and crystallite size with respect to HNO_3 concentration



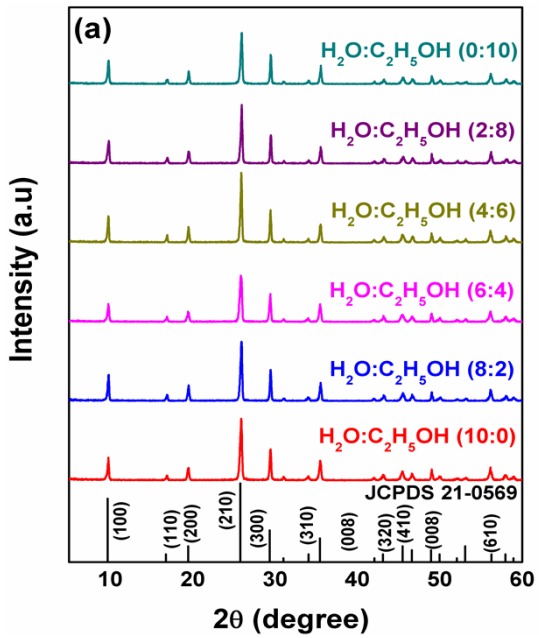
(ESI†) S2 The FT-IR spectra of as-synthesized h-MoO_3 samples prepared with different HNO_3 concentrations

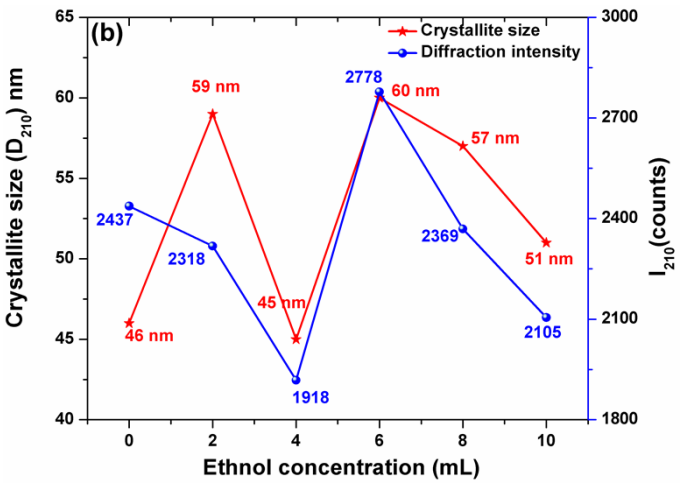


(ESI†) S3(a) XRD patterns of as-synthesized h-MoO_3 sample prepared with different HCl concentrations; **(b)** variation of diffraction peak intensity and crystallite size with respect to HCl concentration

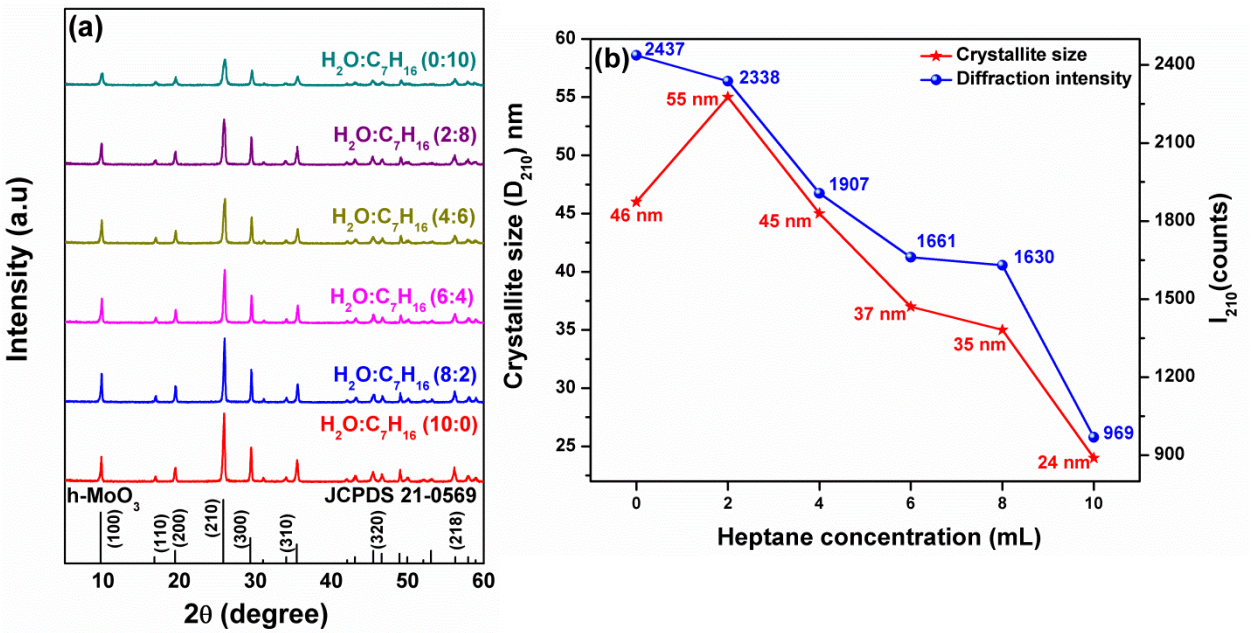


(ESI†) S4 SEM images of as-synthesized h-MoO_3 samples prepared with (a, b) 3 mL; (c, d) 5 mL; (e, f) 10 mL and (g, h) 15 mL HCl concentrations

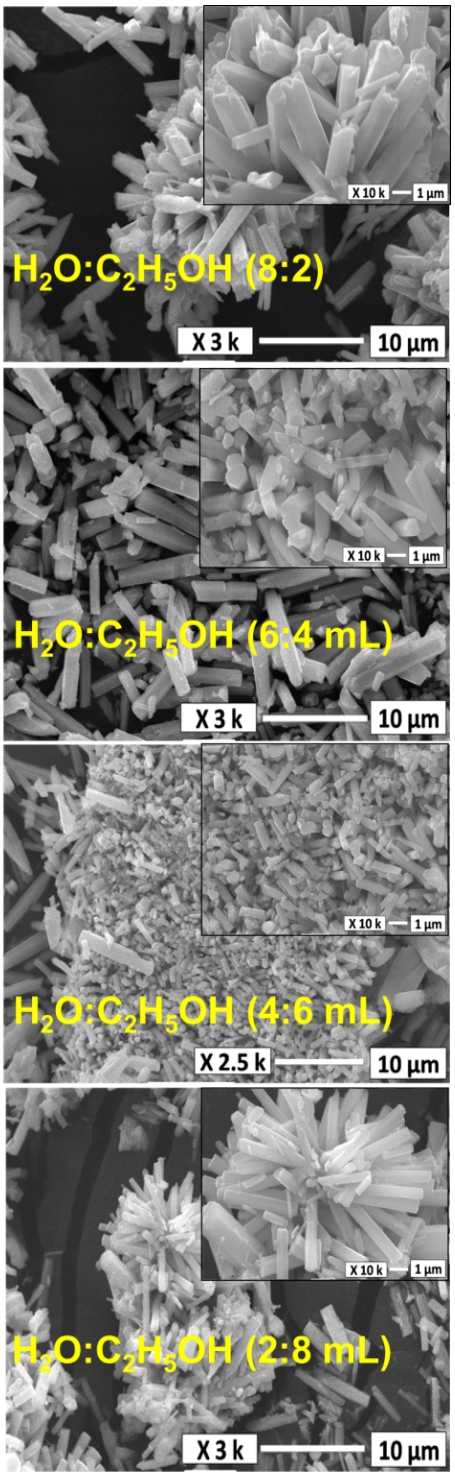

(a)
H2O:C2H5OH (0:10)
H2O:C2H5OH (2:8)
H2O:C2H5OH (4:6)
H2O:C2H5OH (6:4)
H2O:C2H5OH (8:2)
H2O:C2H5OH (10:0)
JCPDS 21-0569
(100)
(110)
(200)
(210)
(300)
(310)
(008)
(320)
(410)
(008)
(610)
Intensity (a.u)
2θ (degree)


(b)
Crystallite size
Diffraction intensity
59 nm
60 nm
57 nm
51 nm
46 nm
45 nm
2437
2318
1918
2778
2369
2105
Crystallite size (D210) nm
I210(counts)
Ethnol concentration (mL)

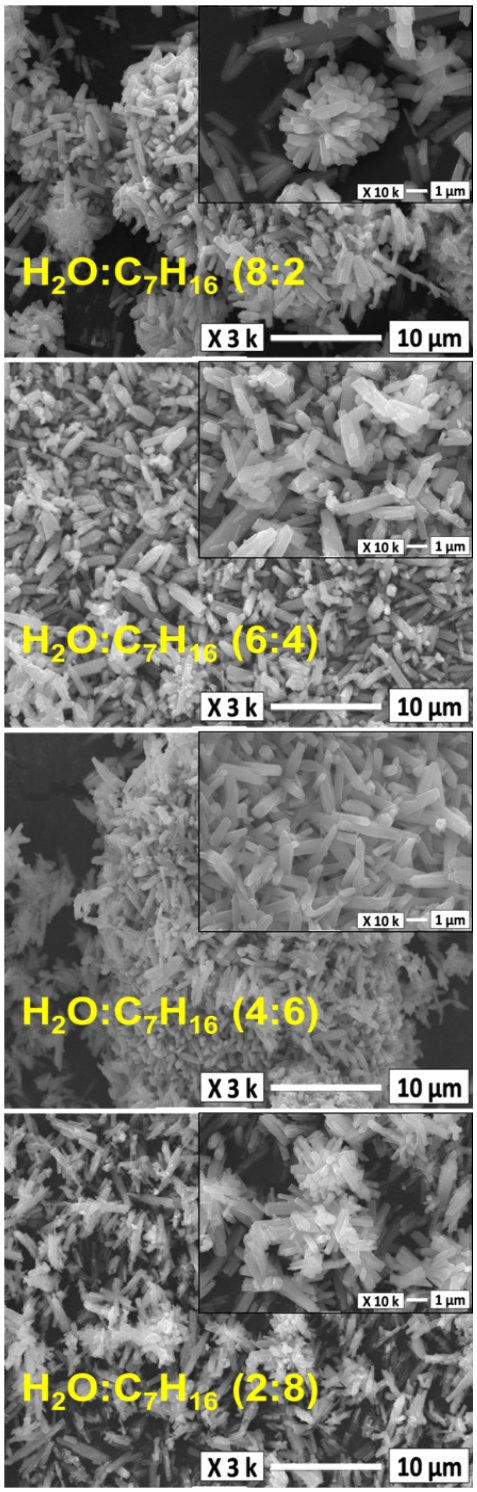
(ESI†) S5(a) XRD pattern of as-synthesized h-MoO_3 samples synthesized using water/ethanol combination; **(b)** variation of diffraction peak intensity and crystallite size with respect to ethanol concentration


(a)
H2O:C7H16 (0:10)
H2O:C7H16 (2:8)
H2O:C7H16 (4:6)
H2O:C7H16 (6:4)
H2O:C7H16 (8:2)
H2O:C7H16 (10:0)
h-MoO3
JCPDS 21-0569
(100)
(110)
(200)
(210)
(300)
(310)
(320)
(218)
Intensity (a.u)
2θ (degree)
(b)
Crystallite size
Diffraction intensity
2437
2338
1907
1661
1630
969
55 nm
46 nm
45 nm
37 nm
35 nm
24 nm
Crystallite size (D210) nm
I210(counts)
Heptane concentration (mL)

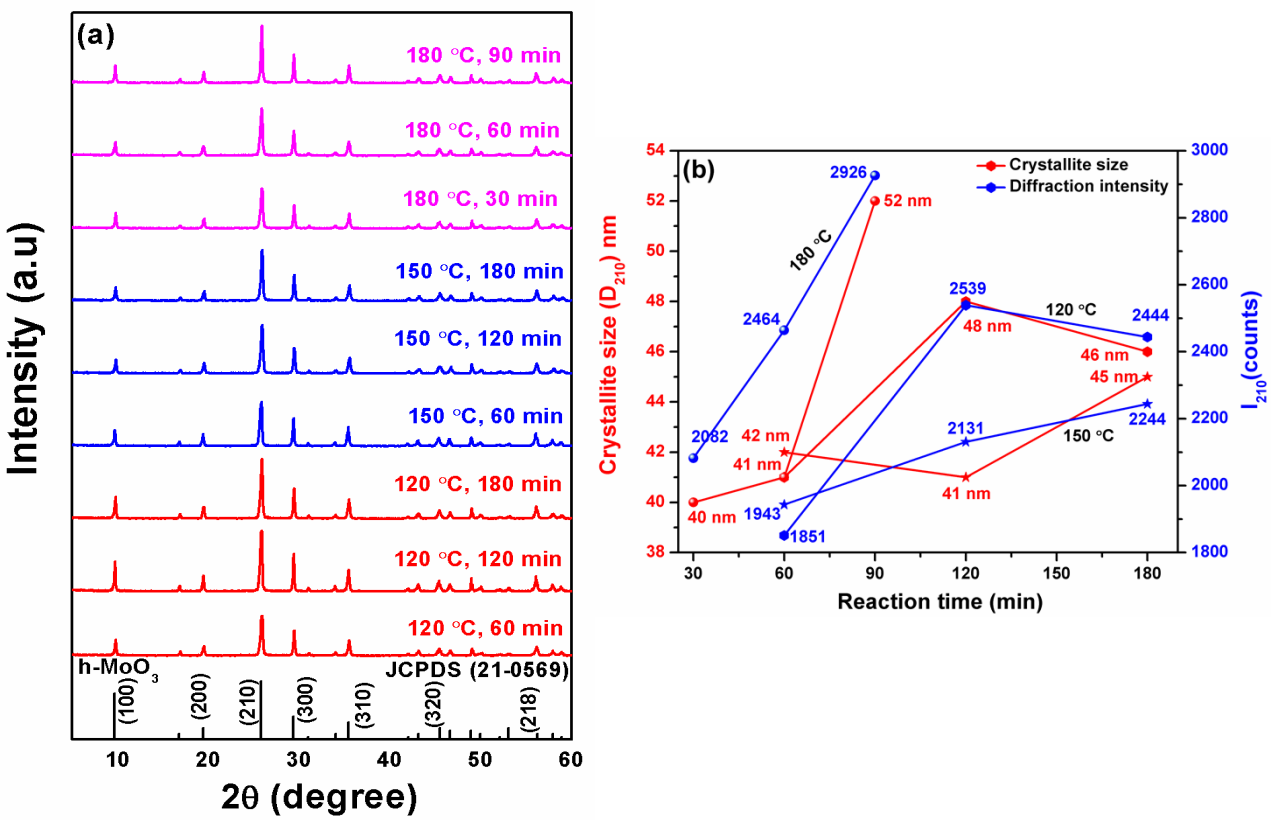
(ESI†) S6(a) XRD pattern of as-synthesized h-MoO_3 samples synthesized using the water / heptane combination; **(b)** variation of diffraction peak intensity and crystallite size with respect to heptane concentration



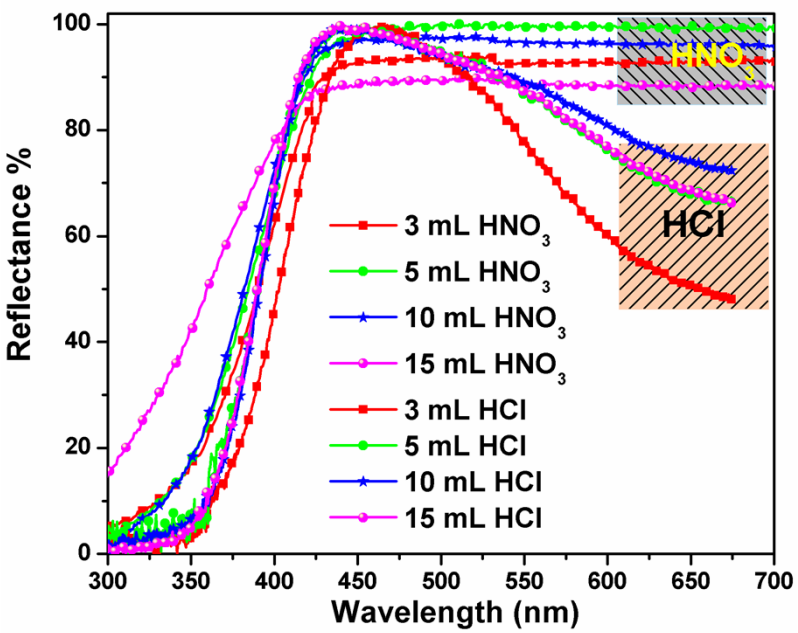
(ESI†) S7 SEM images of as-synthesized h-MoO_3 samples synthesized using water/ethanol compositions



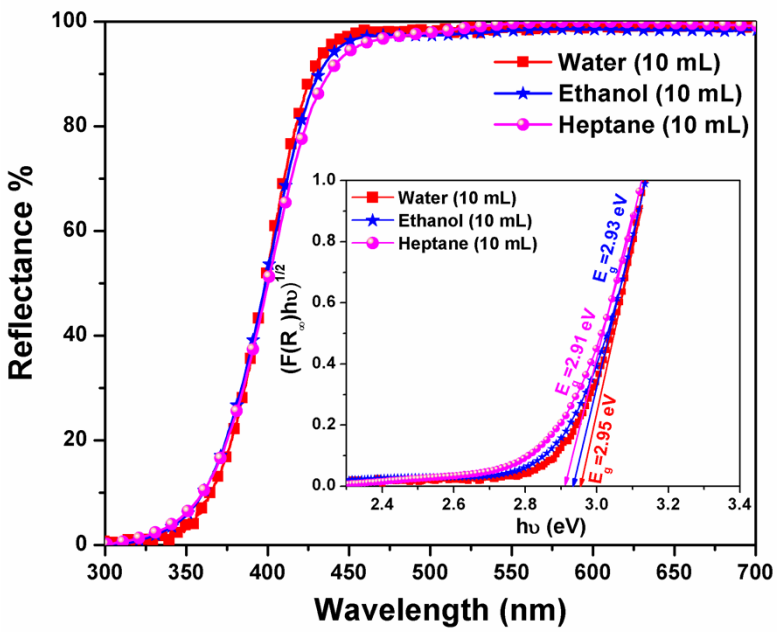
(ESI†) S8 SEM images of as-synthesized h-MoO_3 samples synthesized using water/heptane compositions


(a)
180 °C, 90 min
180 °C, 60 min
180 °C, 30 min
150 °C, 180 min
150 °C, 120 min
150 °C, 60 min
120 °C, 180 min
120 °C, 120 min
120 °C, 60 min
h-MoO3
JCPDS (21-0569)
(100)
(200)
(210)
(300)
(310)
(320)
(218)
Intensity (a.u)
2θ (degree)
(b)
Crystallite size
Diffraction intensity
Crystallite size (D210) nm
I210(counts)
Reaction time (min)
180 °C
120 °C
150 °C
2926
52 nm
2464
2082
42 nm
41 nm
40 nm
1943
1851
2539
48 nm
2444
46 nm
45 nm
2131
41 nm
2244

(ESI†) S9(a) XRD patterns of h-MoO_3 samples synthesized at different reaction time and reaction temperature; **(b)** Variation of diffraction peak intensity and crystallite size with respect to reaction time and reaction temperature



(ESI†) S10 UV-Vis diffuse reflectance spectra of samples obtained for different HNO_3 and HCl concentrations



(ESI†) S11 UV-Vis diffuse reflectance spectra of as-synthesized h-MoO_3 samples synthesized under water, ethanol and heptane as solvent medium; inset shows the band gap of h-MoO_3