Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

An insight into the origin of room-temperature ferromagnetism in SnO_2 and Mn -doped SnO_2 quantum dots: an experimental and DFT approach

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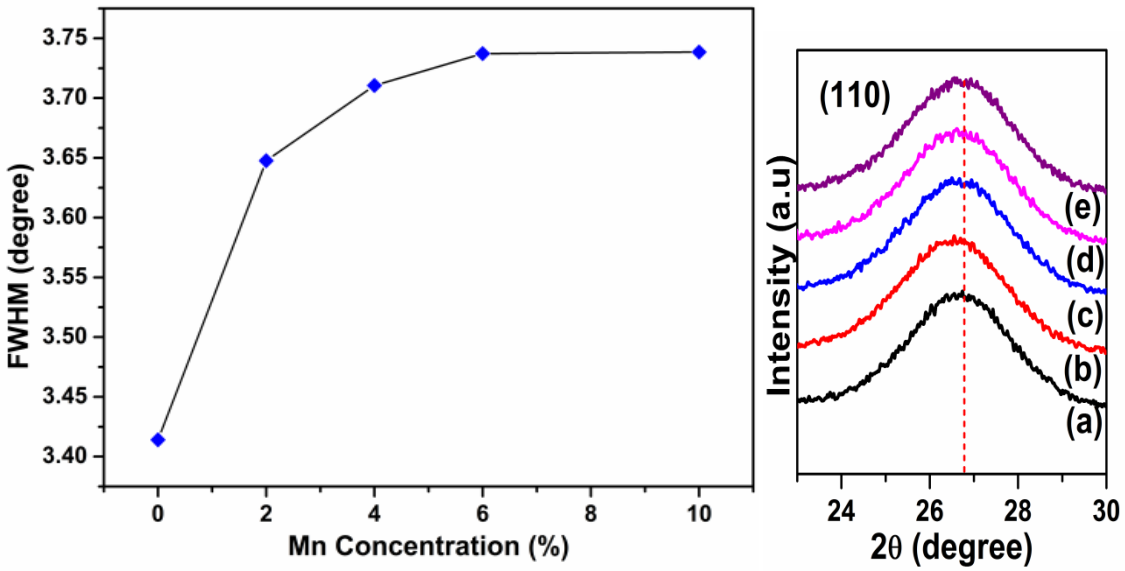
Supporting Information

1. FWHM of (110) diffraction peak as a function of Mn concentration and magnified diffraction peak (110).

2. Lattice parameters as a function of Mn concentration with error bars (Graphical representation).

3. Deconvoluted room temperature Raman spectra.

4. Temperature dependent Raman spectra and temperature dependence of classical Raman modes.



(A) **(B)**

Fig. S1 (A) FWHM of (110) diffraction peak as a function of Mn concentration (B) Magnified diffraction peak (110) a) Undoped SnO_2 b) 2% Mn doped SnO_2 c) 4% Mn doped SnO_2 d) 6% Mn doped SnO_2 and e) 10% Mn doped SnO_2 QDs.

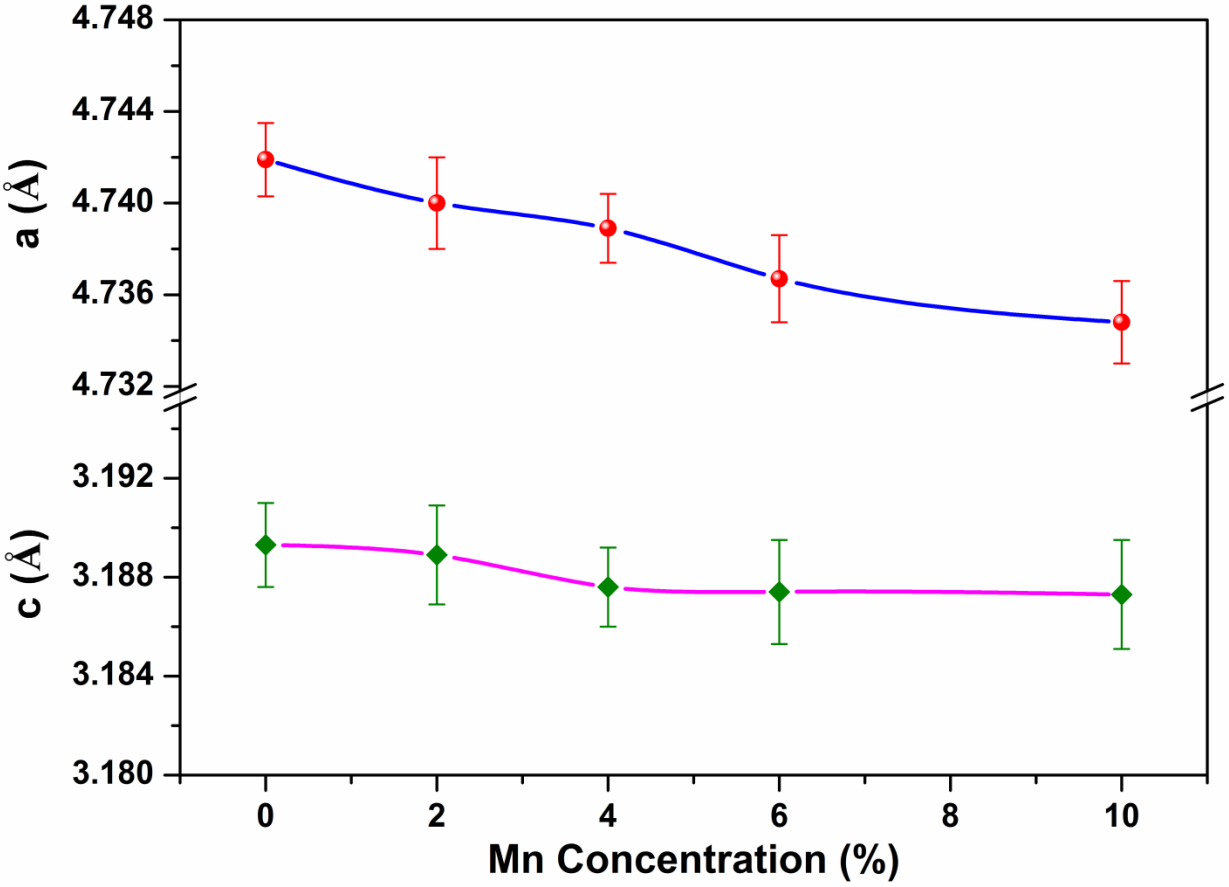
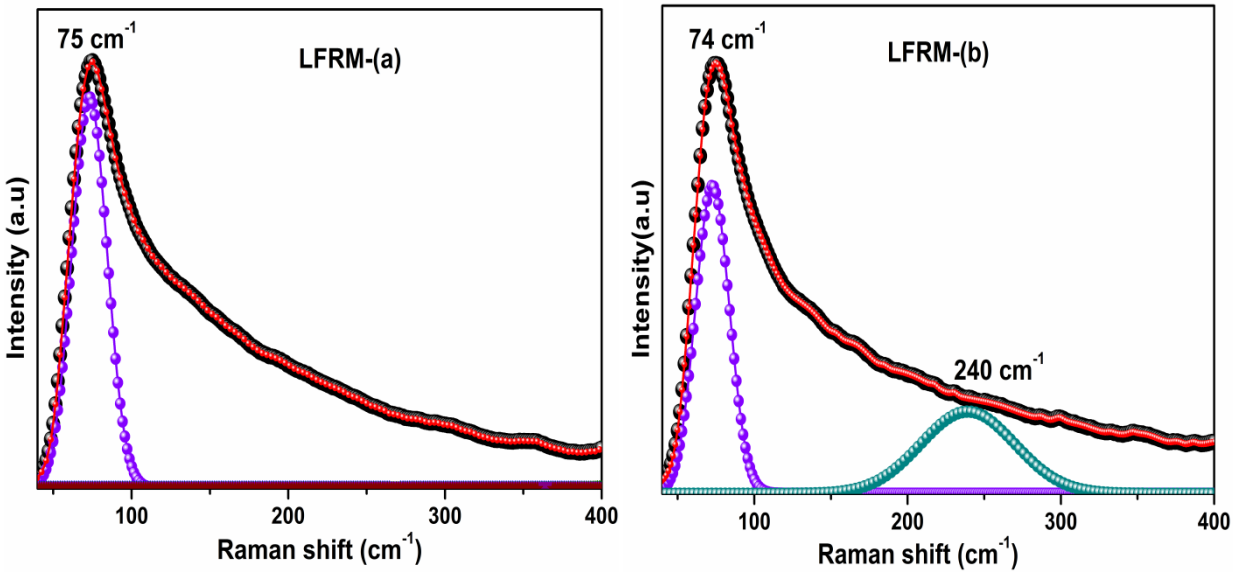


Fig. S2 Lattice parameter as a function of Mn concentration with error bars.


75 cm-1
LFRM-(a)
Intensity (a.u)
100
200
300
400
Raman shift (cm-1)
74 cm-1
LFRM-(b)
Intensity(a.u)
240 cm-1
100
200
300
400
Raman shift (cm-1)

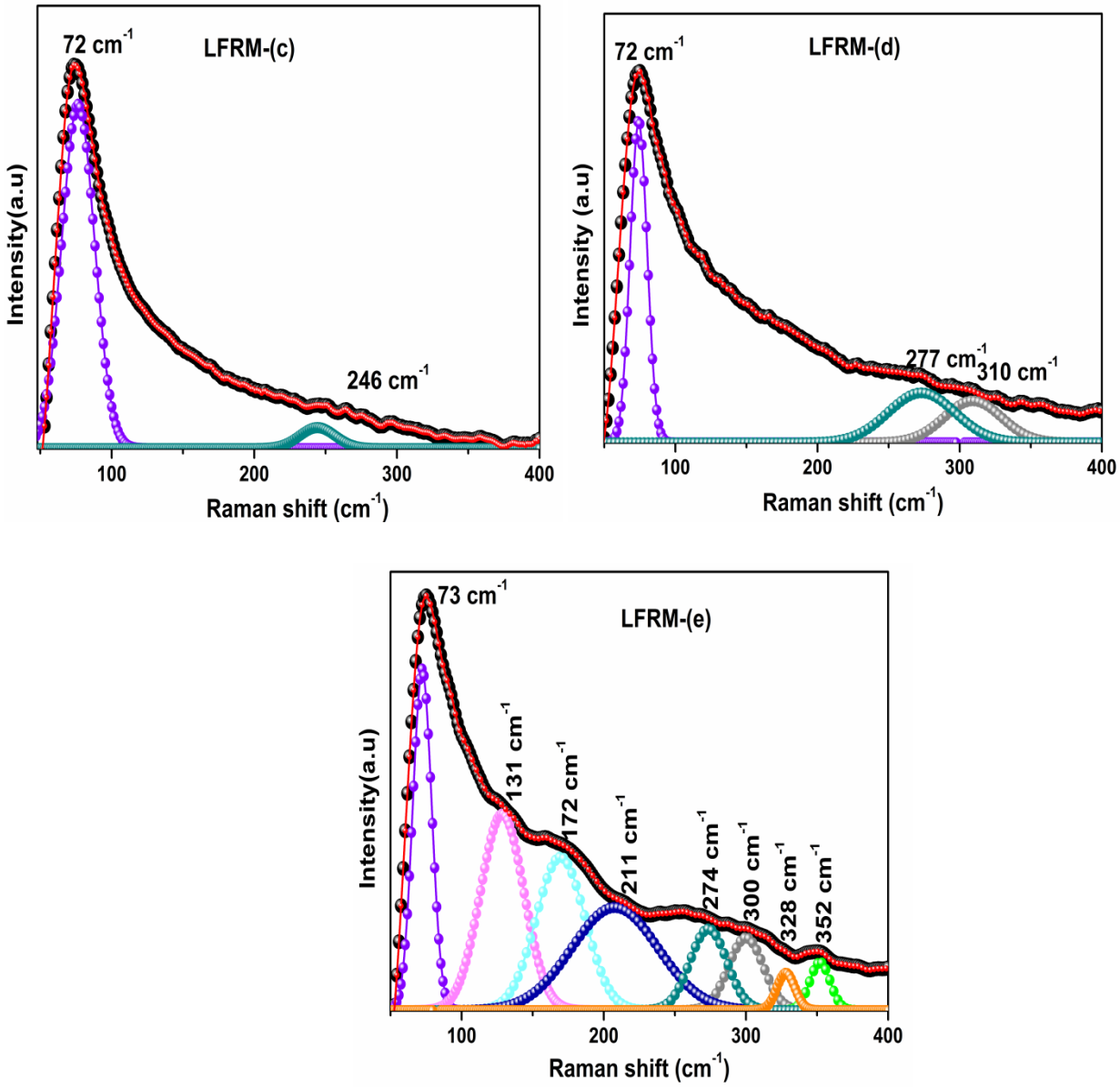
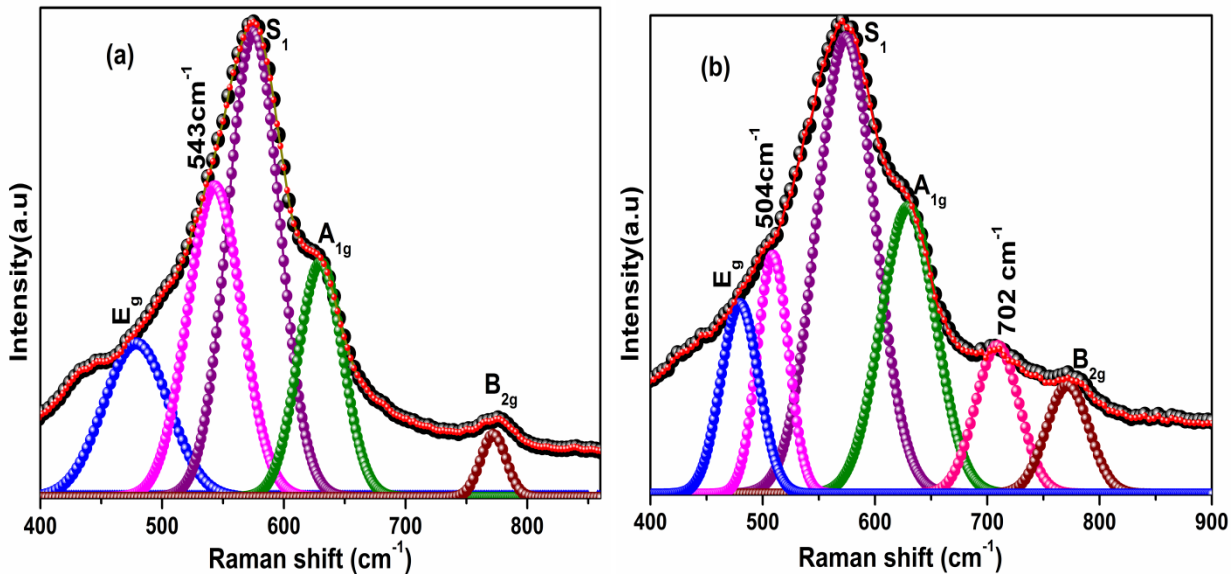


Fig. S3 Deconvoluted room temperature Raman spectra measured in the region 50-400 $cm^{-1}$of a) Undoped SnO_2 and b) 2% Mn doped SnO_2 c) 4% Mn doped SnO_2 d) 6% Mn doped SnO_2 and e) 10% Mn doped SnO_2 QDs.


(a)
S1
543cm-1
A1g
Eg
B2g
Intensity(a.u)
400
500
600
700
800
Raman shift (cm-1)
(b)
S1
504cm-1
A1g
Eg
702 cm-1
B2g
Intensity(a.u)
400
500
600
700
800
900
Raman shift (cm-1)

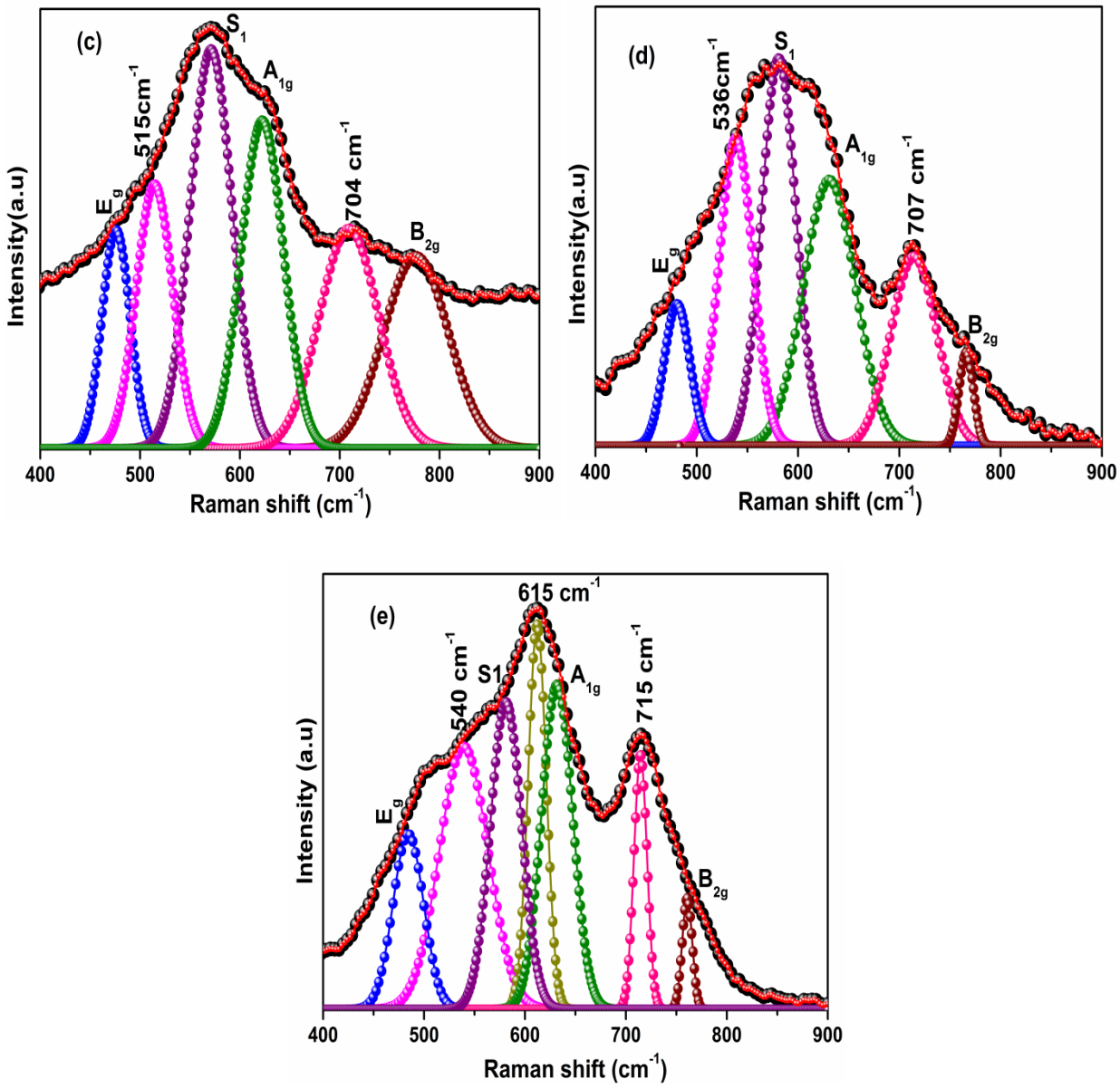
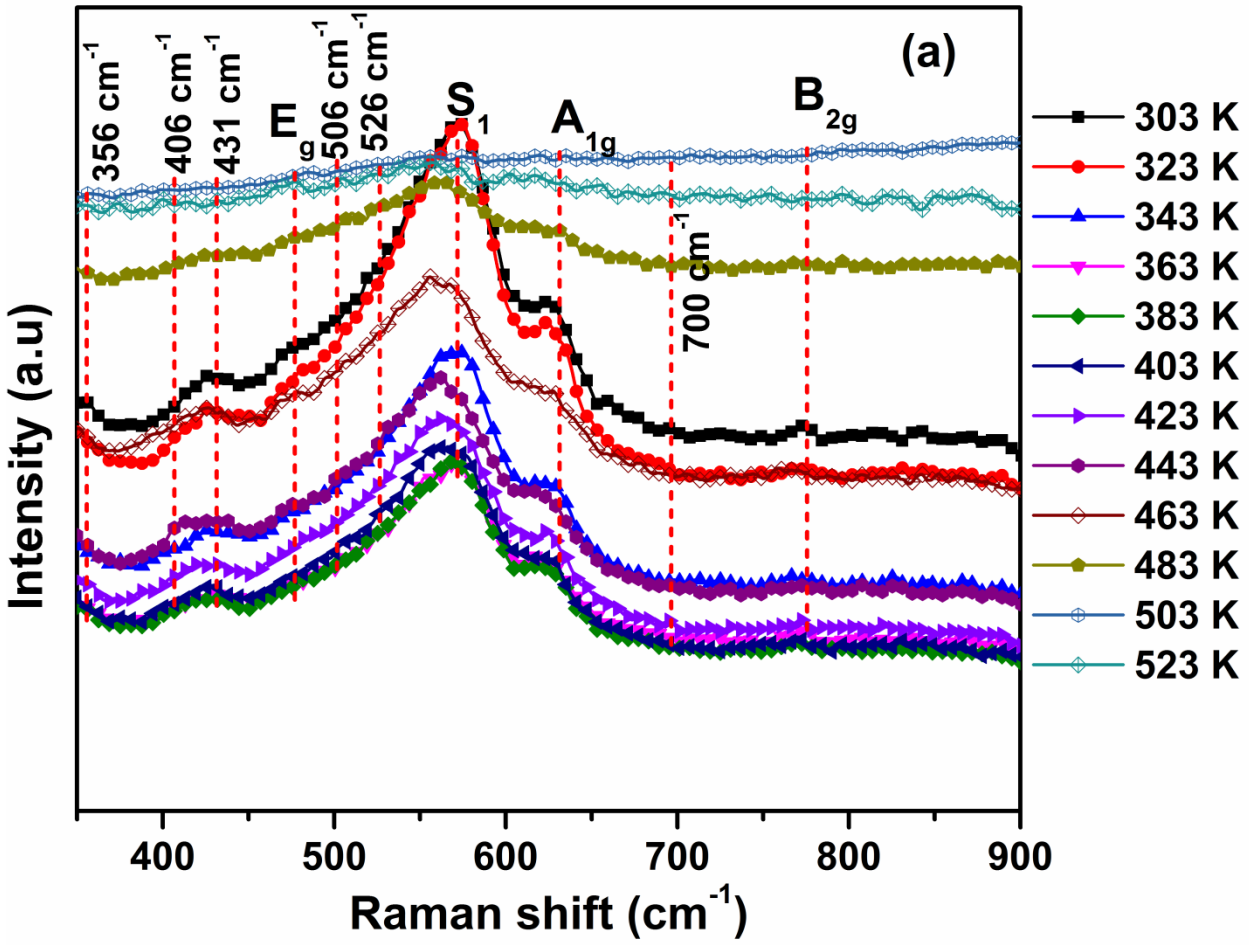
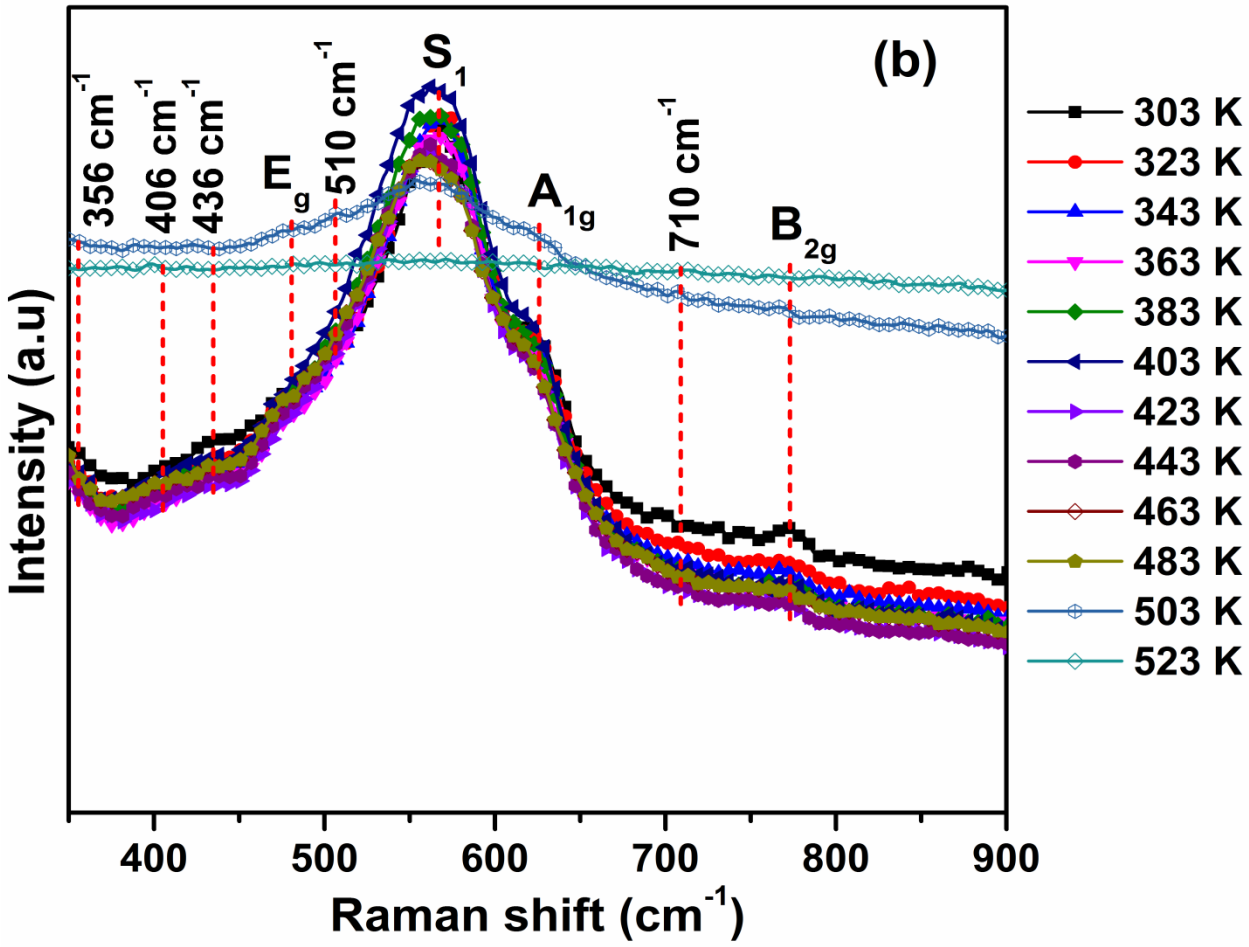
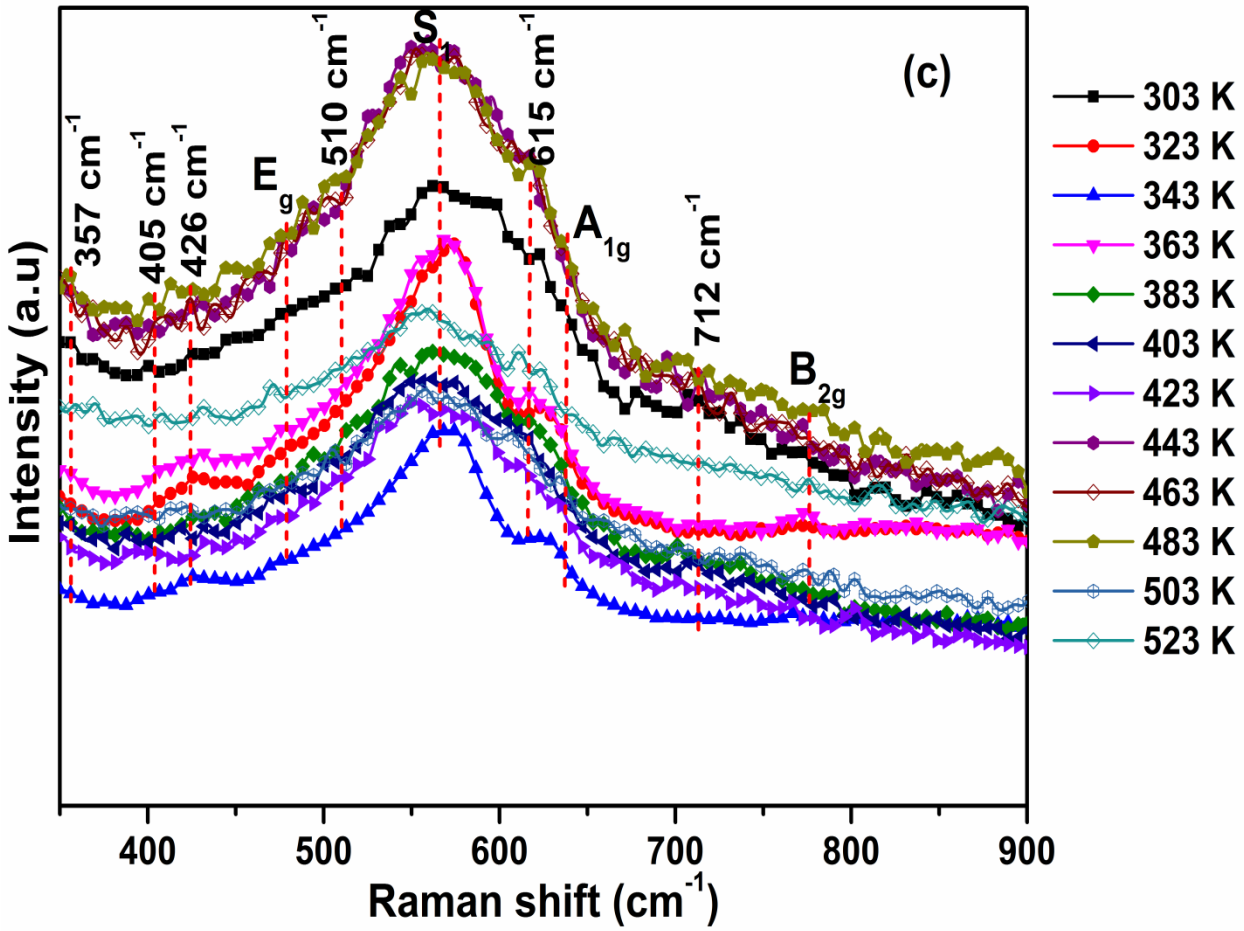
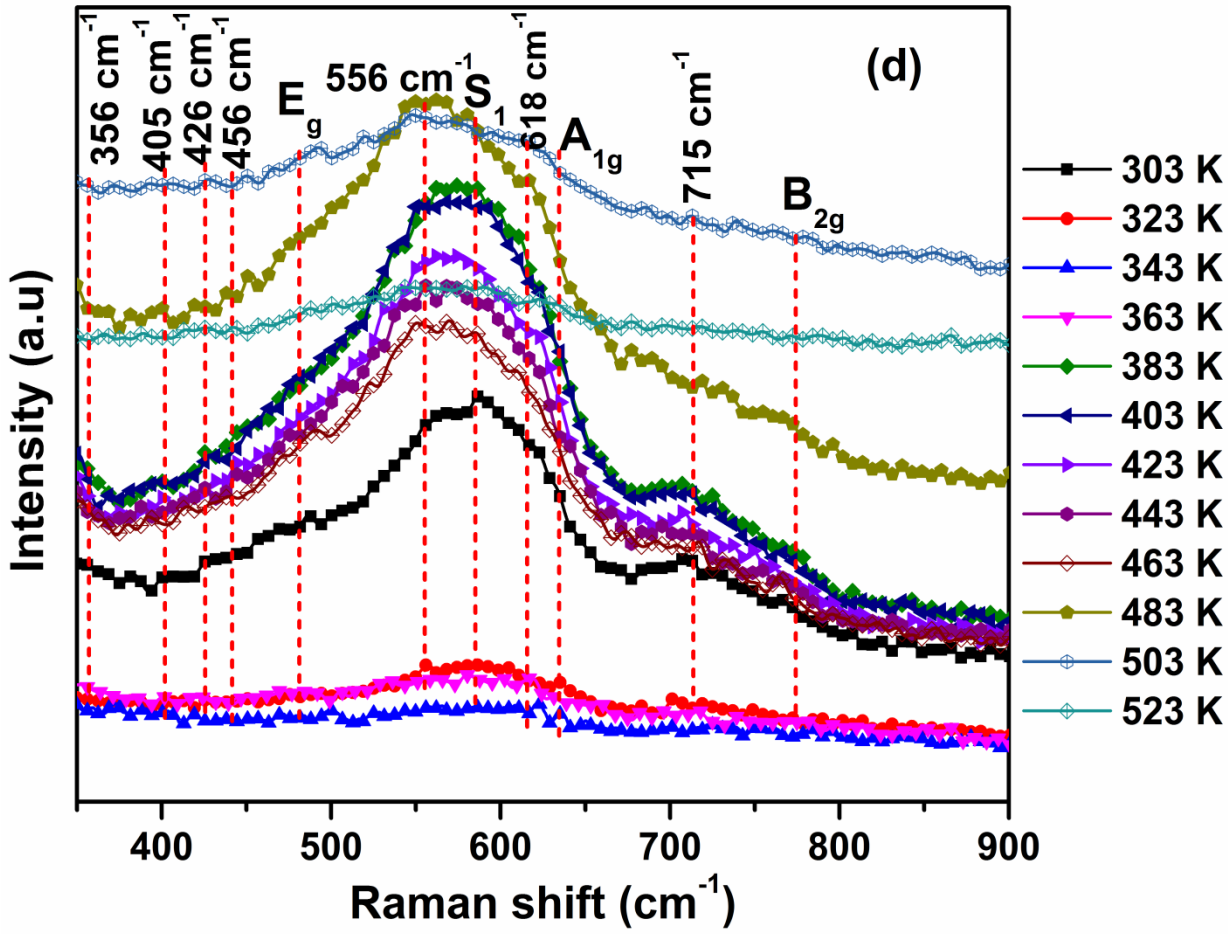


Fig. S4 Deconvoluted room temperature Raman spectra measured in the region 400-900 cm^{-1} of a) Undoped SnO_2 and b) 2% Mn doped SnO_2 c) 4% Mn doped SnO_2 d) 6% Mn doped SnO_2 and e) 10% Mn doped SnO_2 QDs.


(a)
356 cm-1
406 cm-1
431 cm-1
Eg
506 cm-1
526 cm-1
S1
A1g
700 cm-1
B2g
303 K
323 K
343 K
363 K
383 K
403 K
423 K
443 K
463 K
483 K
503 K
523 K
Intensity (a.u)
400
500
600
700
800
900
Raman shift (cm-1)


(b)
356 cm-1
406 cm-1
436 cm-1
Eg
510 cm-1
S1
A1g
710 cm-1
B2g
Intensity (a.u)
400
500
600
700
800
900
Raman shift (cm-1)
303 K
323 K
343 K
363 K
383 K
403 K
423 K
443 K
463 K
483 K
503 K
523 K


(c)
357 cm-1
405 cm-1
426 cm-1
Eg
510 cm-1
S
615 cm-1
A1g
712 cm-1
B2g
Intensity (a.u)
Raman shift (cm-1)
400
500
600
700
800
900
303 K
323 K
343 K
363 K
383 K
403 K
423 K
443 K
463 K
483 K
503 K
523 K


(d)
356 cm-1
405 cm-1
426 cm-1
456 cm-1
Eg
556 cm-1
S1
618 cm-1
A1g
715 cm-1
B2g
303 K
323 K
343 K
363 K
383 K
403 K
423 K
443 K
463 K
483 K
503 K
523 K
Intensity (a.u)
400
500
600
700
800
900
Raman shift (cm-1)

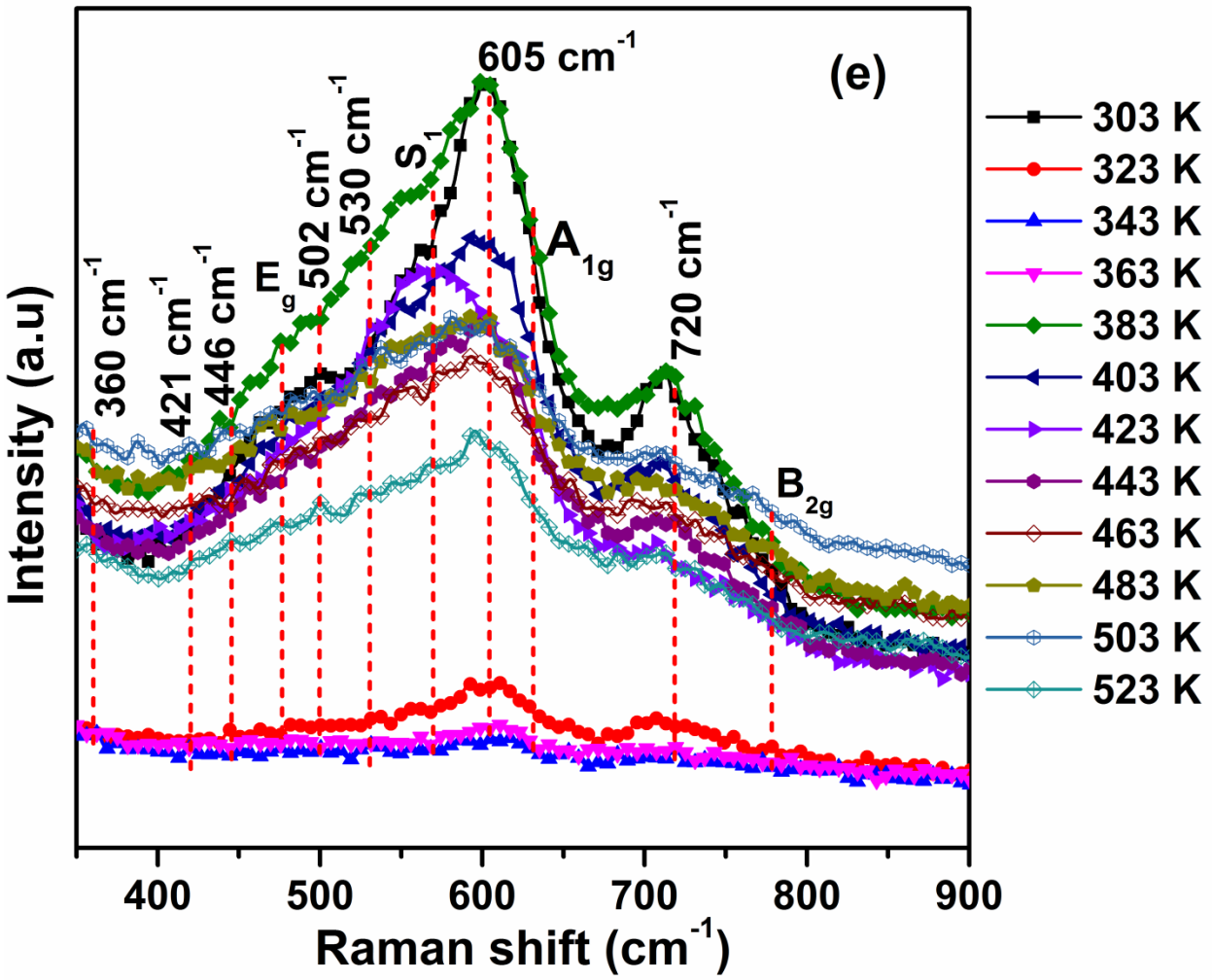
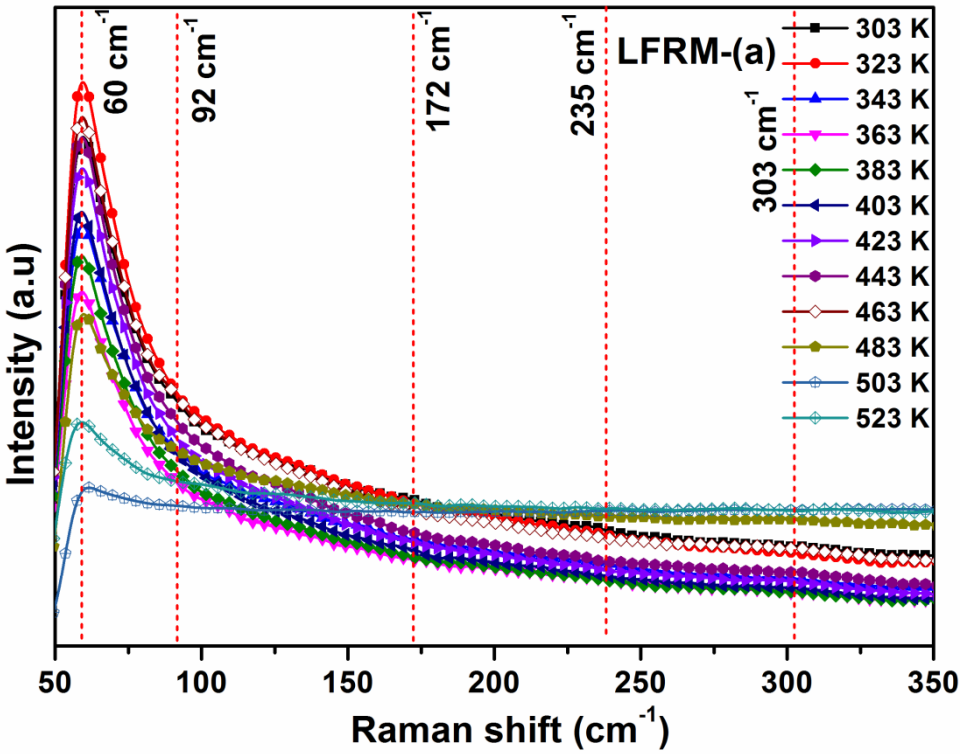
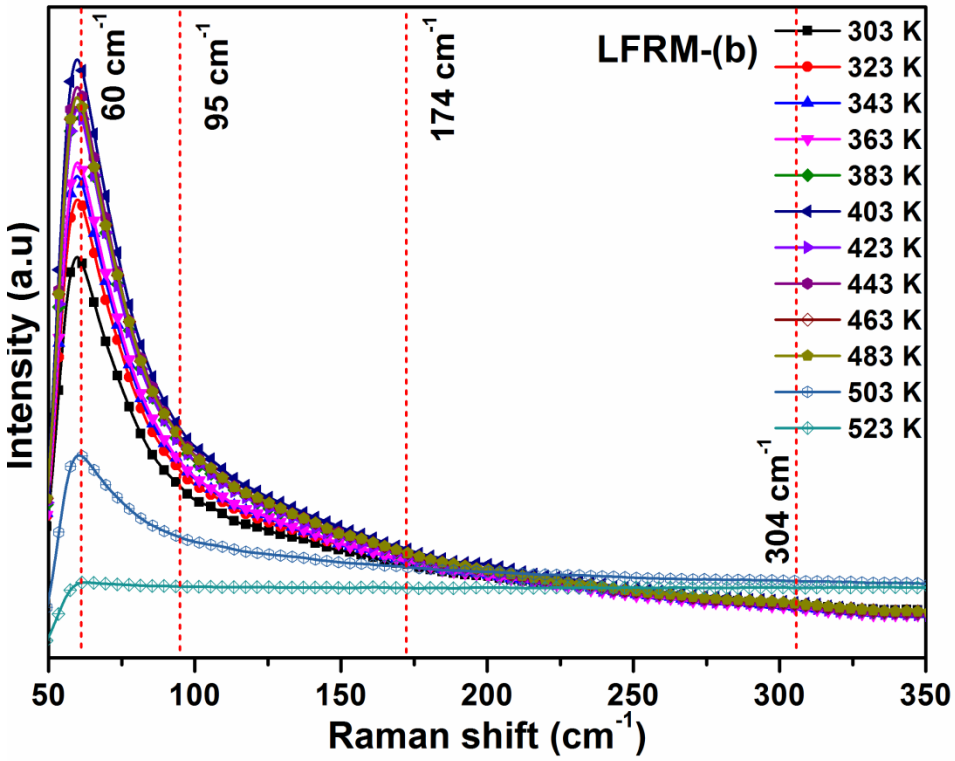
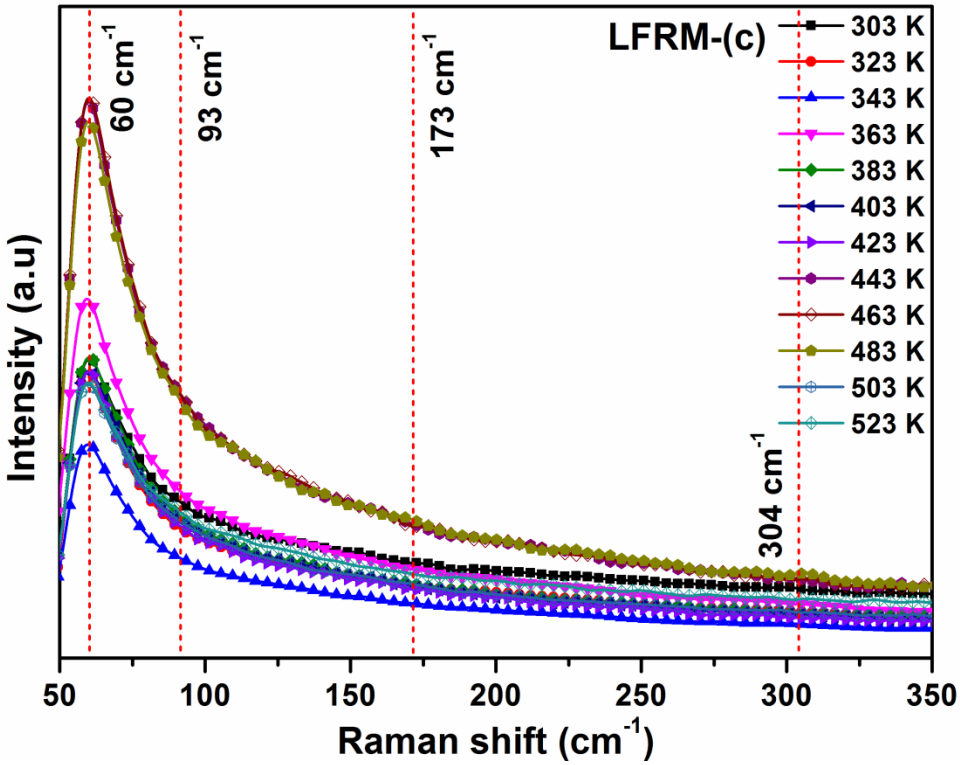
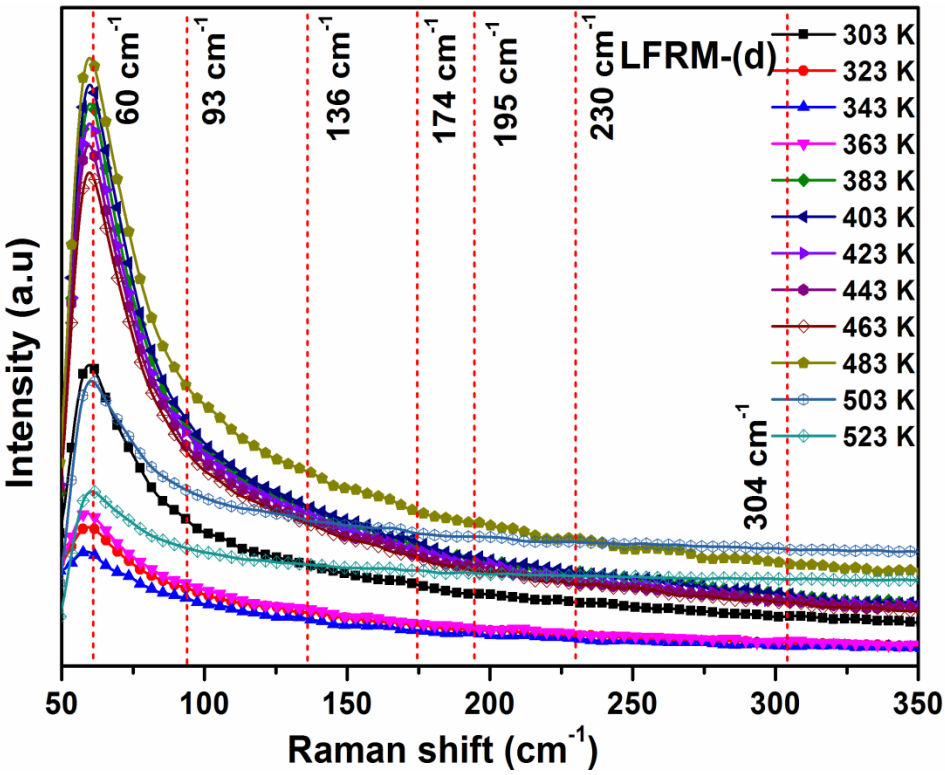


Fig. S5 Temperature dependent Raman spectra measured in the region 350-900 cm^{-1} of a) Undoped SnO_2 and b) 2% Mn doped SnO_2 c) 4% Mn doped SnO_2 d) 6% Mn doped SnO_2 and e) 10% Mn doped SnO_2 QDs.


60 cm-1
92 cm-1
172 cm-1
235 cm-1
303 cm-1
LFRM-(a)
303 K
323 K
343 K
363 K
383 K
403 K
423 K
443 K
463 K
483 K
503 K
523 K
Intensity (a.u)
50
100
150
200
250
300
350
Raman shift (cm-1)


LFRM-(b)
60 cm-1
95 cm-1
174 cm-1
304 cm-1
303 K
323 K
343 K
363 K
383 K
403 K
423 K
443 K
463 K
483 K
503 K
523 K
Intensity (a.u)
Raman shift (cm-1)
50
100
150
200
250
300
350


LFRM-(c)
60 cm-1
93 cm-1
173 cm-1
304 cm-1
303 K
323 K
343 K
363 K
383 K
403 K
423 K
443 K
463 K
483 K
503 K
523 K
Intensity (a.u)
Raman shift (cm-1)
50
100
150
200
250
300
350


LFRM-(d)
60 cm-1
93 cm-1
136 cm-1
174 cm-1
195 cm-1
230 cm-1
304 cm-1
303 K
323 K
343 K
363 K
383 K
403 K
423 K
443 K
463 K
483 K
503 K
523 K
Intensity (a.u)
Raman shift (cm-1)
50
100
150
200
250
300
350

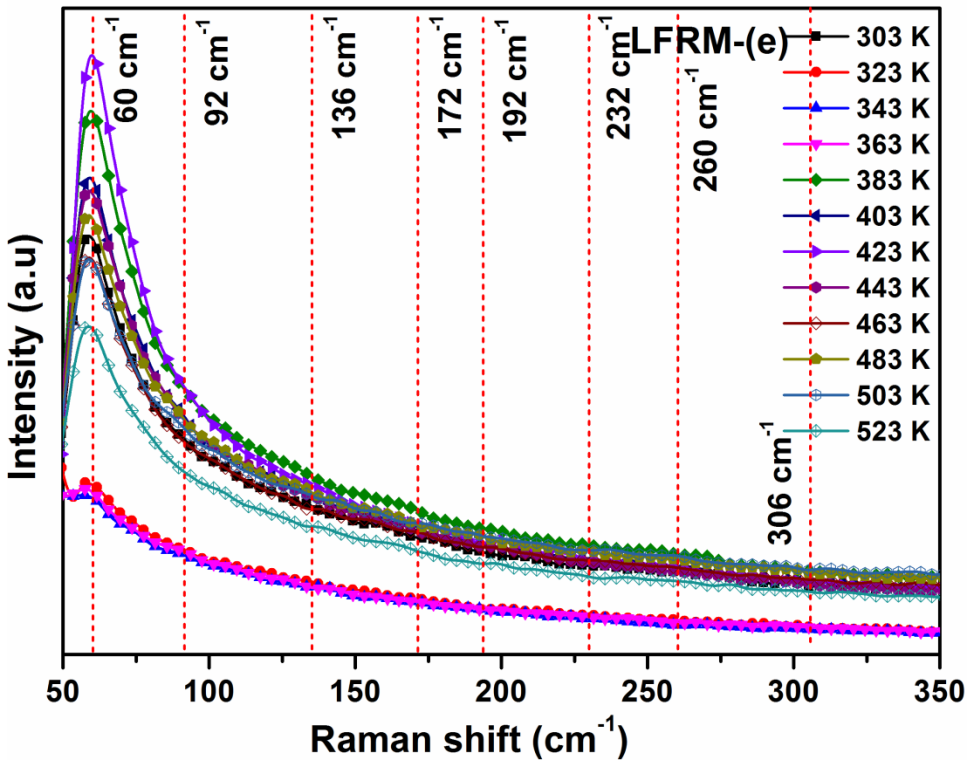


Fig. S6 Temperature dependent Raman spectra measured in the region 50-350 cm^{-1} of a) Undoped SnO_2 and b) 2% Mn doped SnO_2 c) 4% Mn doped SnO_2 d) 6% Mn doped SnO_2 and e) 10% Mn doped SnO_2 QDs.

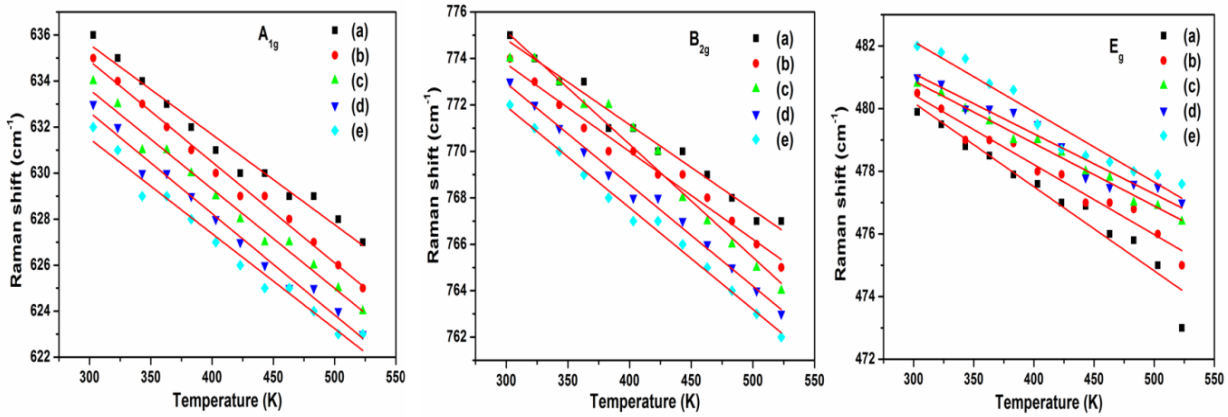


Fig. S7 Temperature dependence of classical Raman modes of a) Undoped SnO_2 b) 2% Mn doped SnO_2 c) 4% Mn doped SnO_2 d) 6% Mn doped SnO_2 and e) 10% Mn doped SnO_2 QDs. (scatter points are experimental data and red line represents fitting using straight line equation (3))