

## **Supporting information**

# **Impact of Mn-Dopant Concentration in Observing Narrowing of Band-Gap, Urbach tail and Paramagnetism in Anatase TiO<sub>2</sub> Nanocrystals**

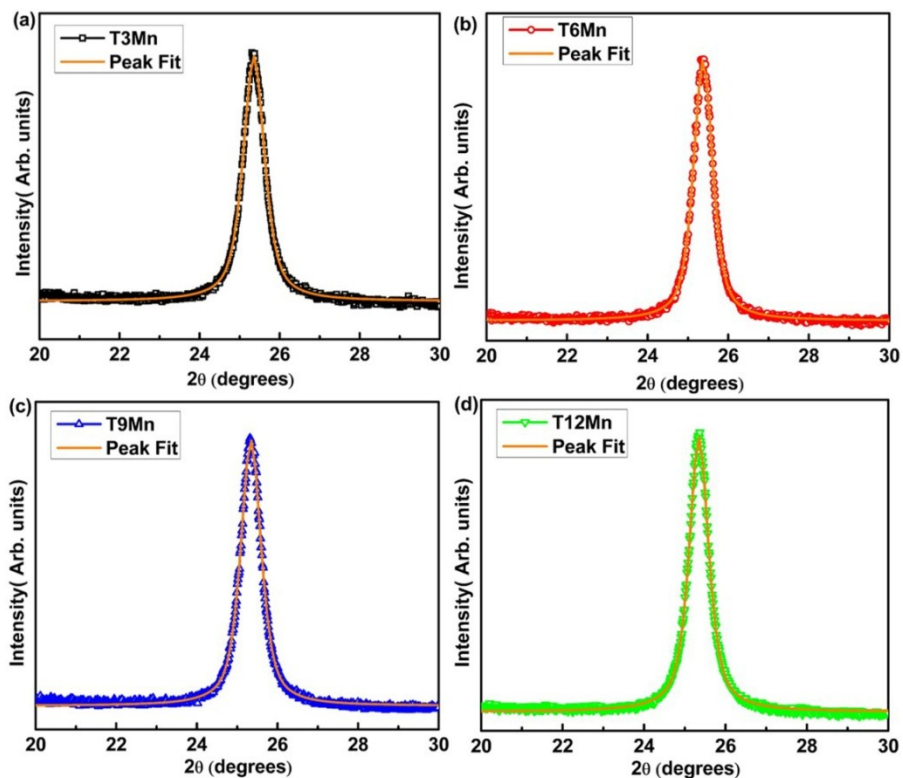
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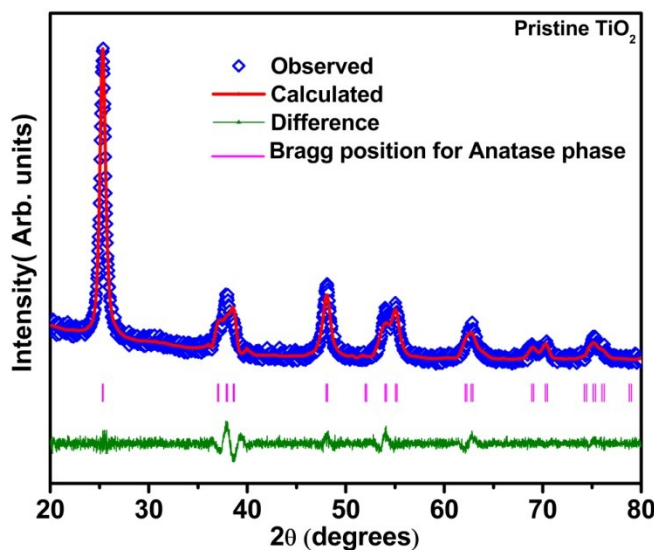
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**Fig.S1:** Estimation of FWHM from the most intense (101) peak of all the Mn-doped samples (a) T3Mn, (b) T6Mn, (c) T9Mn and (d) T12Mn



**Figure S2.** Refined XRD patterns of Pristine TiO<sub>2</sub> nanocrystals

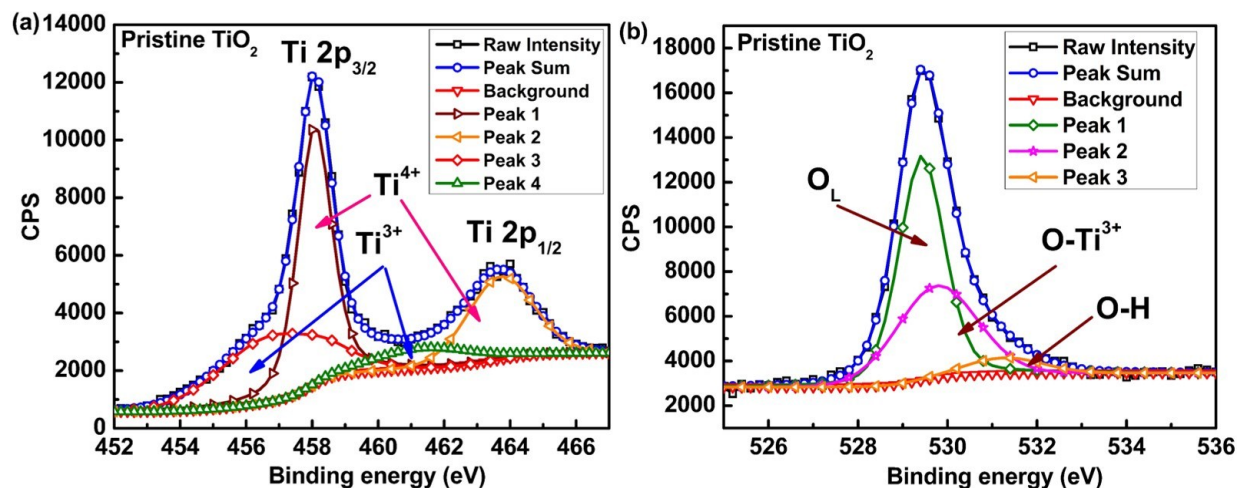


Figure S3. (a) High resolution XPS spectra of (a) Ti 2p and (b) O 1s of Pristine TiO<sub>2</sub>

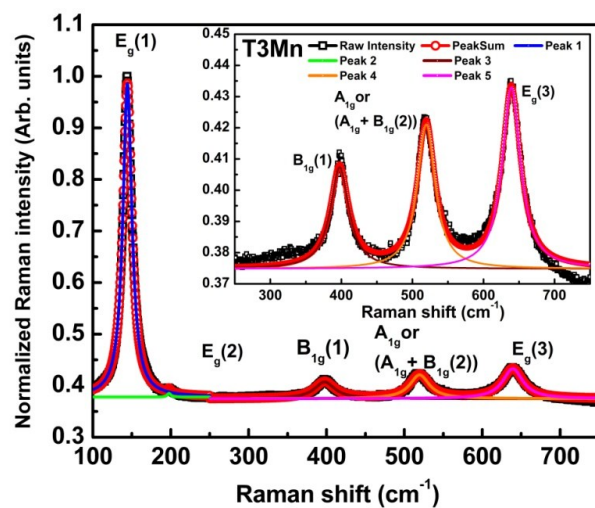


Figure S4: Deconvoluted Raman spectra of 3% Mn-doped TiO<sub>2</sub>

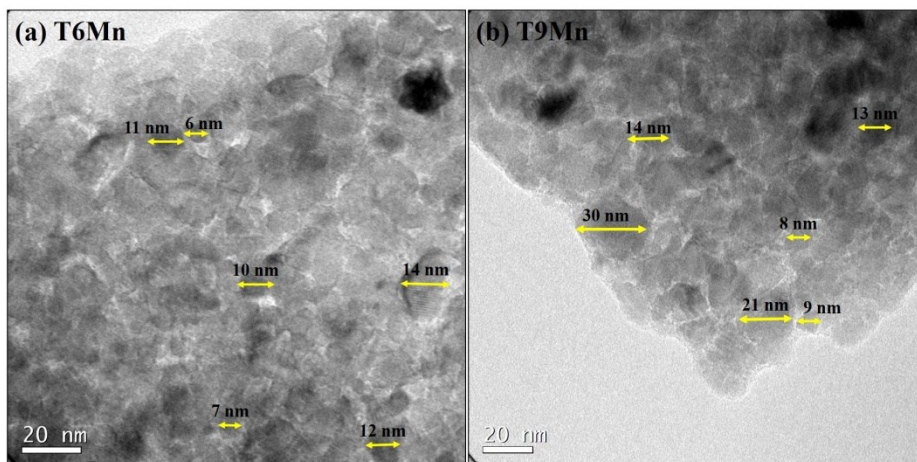
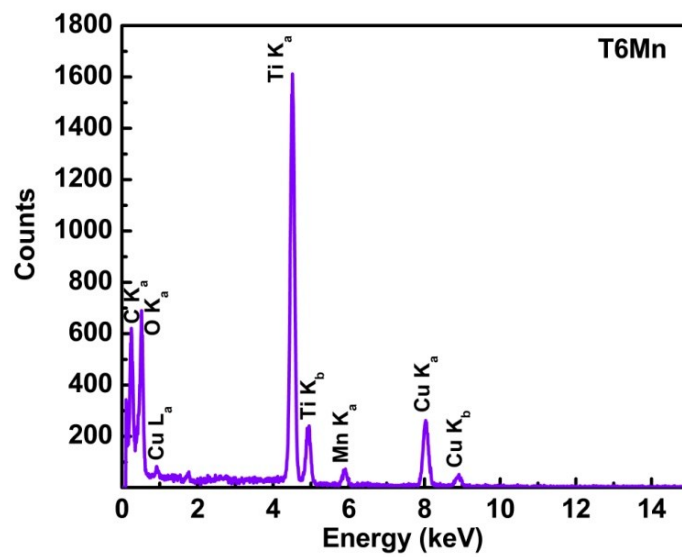


Figure S5: TEM micrographs showing the nanocrystal formation for (a) T6Mn and (b) T9Mn



**Figure S6:** EDS spectra of 6% Mn-doped TiO<sub>2</sub> as a representative of the series

**Table S1:** Refinement parameters obtained for undoped and Mn-doped TiO<sub>2</sub> nanocrystals

<b>Compound</b>	<b>Pristine TiO<sub>2</sub></b>	<b>T3Mn</b>	<b>T6Mn</b>	<b>T9Mn</b>	<b>T12Mn</b>
<b>Phase</b>	Anatase				
<b>Crystal Structure</b>	Tetragonal				
<b>Space Group</b>	I 41/a m d				
<b>Lattice Parameters</b>					
<b>a(Å)</b>	3.7901(1)	3.7907(4)	3.7911(1)	3.7923(4)	3.7953(5)
<b>c(Å)</b>	9.4923(3)	9.4926(2)	9.4928(1)	9.5136(3)	9.5035(4)
<b>Volume (Å)<sup>3</sup></b>	136.35(2)	136.40(3)	136.43(2)	136.82(6)	136.89(1)
<b>Atomic positions</b>					
<b>Ti/Mn<sub>x</sub> (4a)</b>	0.0000	0.0000	0.0000	0.0000	0.0000
<b>Ti/Mn<sub>y</sub> (4a)</b>	0.7500	0.7500	0.7500	0.7500	0.7500
<b>Ti/Mn<sub>z</sub> (4a)</b>	0.1250	0.1250	0.1250	0.1250	0.1250
<b>O<sub>x</sub> (8e)</b>	0.0000	0.0000	0.0000	0.0000	0.0000
<b>O<sub>y</sub> (8e)</b>	0.2500	0.2500	0.2500	0.2500	0.2500
<b>O<sub>z</sub> (8e)</b>	0.0835(5)	0.0762(9)	0.0755(2)	0.0788(8)	0.0712(1)
<b>B<sub>iso</sub> (Ti/Mn) (Å)<sup>2</sup></b>	0.0009	0.0158	0.0197	0.0261	0.0205
<b>B<sub>iso</sub> (O) (Å)<sup>2</sup></b>	0.0075	0.0789	0.0861	0.0324	0.0576
<b>Occ (Ti)</b>	0.1250	0.1213	0.1175	0.1137	0.1100
<b>Occ (Mn)</b>	-	0.0037	0.0075	0.0112	0.0150
<b>Occ (O)</b>	0.1250	0.1250	0.1250	0.1250	0.1250
<b>Residual Parameters</b>					
<b>R<sub>p</sub></b>	4.56	3.68	3.51	3.55	2.98
<b>R<sub>wp</sub></b>	5.77	5.15	4.79	4.85	3.90
<b>χ<sup>2</sup></b>	1.89	1.49	1.22	1.15	1.55

**Table S2:** Variation of FWHM with Mn doping for all the samples

<b>Sample</b>	<b>FWHM</b>
TP	0.63612
T3Mn	0.62970
T6Mn	0.60726
T9Mn	0.57399
T12Mn	0.56651

**Table S3:** ED-XRFS results showing Ti:Mn ratio for all the Mn-doped TiO<sub>2</sub> nanocrystals

<b>Sample</b>	<b>TiO<sub>2</sub> (%)</b>	<b>MnO (%)</b>	<b>Ti:Mn (Nominal)</b>	<b>Ti:Mn (Real)</b>
T3Mn	97.15	2.85	32.33	30.26
T6Mn	94.31	5.69	15.67	14.72
T9Mn	91.28	8.72	10.11	9.30
T12Mn	88.47	11.53	7.33	6.82