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Supporting Information

Non-uniform distribution of dopant iron ions in TiO₂ nanocrystals probed by X-ray diffraction, Raman scattering, photoluminescence and photocatalysis

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Table S1 Variation of intensities of XRD peaks with doping % of Fe. Ratio of intensities of peaks in the XRD patterns of doped samples relative to the intensity of corresponding peaks in the pattern of undoped sample. I_{d1} , I_{d2} and I_{d3} are the intensity of the most intense, second most intense and third most intense peak of Fe doped sample; I_{d01} , I_{d02} and I_{d03} are the intensity of the most intense, second most intense and third most intense.

Doping % of	Id1/Id01	Id2/Id02	Id3/Id03
iron			
1	0.9331	0.9431	0.9595
2	0.8135	0.8240	0.7911
5	0.7705	0.7928	0.8180
8	0.48869	0.4983	0.4756

X-ray Diffraction



Fig. S1 X-Ray diffraction patterns of samples F15, F20*, F25* and F25 (inset). All the XRD peaks of F15 except the one at 2 θ value of 25.3°, which is the strongest (101) peak of anatase, are associated with rutile phase of TiO₂. Nanocrystalline TiO₂ samples doped with 20 and 25 atom % of Fe and annealed at 600°C show amorphous structure (inset, XRD pattern of F25). But when the two samples are annealed at 800°C for 1 hour (F20* and F25*), the XRD patterns show peaks of F15 along with new peaks. All the new peaks in the XRD patterns of F20* and F25* are identified as peaks belonging to iron titanium oxide (pseudobrookite).



1% Fe-doped TiO₂

2% Fe-doped TiO₂

Fig. S2 TEM micrographs of nanocrystals of TiO_2 containing 1 atom % and 2 atom % of iron.





Fig. S3 Micro-Raman spectra of samples F15, F20*, and F25*. The spectrum of F15 showed amorphous pattern with the most intense Raman line of anatase appearing around 150 cm⁻¹. The spectra of F20* and F25* show the characteristic Raman peaks of iron titanium oxide appearing at 199, 222, and 335 cm⁻¹. Fig. shows that the intensity of the peaks decreased rapidly with increase in the atom % of iron in the samples.

Optical Absorption Spectra



Fig. S4 Optical absorption spectra of iron doped nanoparticles of TiO_2 . The absorption edge shifted regularly towards longer wave lengths as doping concentration of Fe increased. The band gap is the smallest for F25* containing the highest concentration.

Photoluminescence Spectra



Fig. S5 Photoluminescence spectra of 1% iron doped nanoparticles of TiO_2 at three excitation wavelengths.