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Particle
& Particle Systems Characterization

Supporting Information

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Highly Selective Optical Detection of Fe^{3+} Ions in Aqueous Solution Using Label-Free Silicon Nanocrystals

*Keith Linehan, Darragh Carolan, and Hugh Doyle**

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Supporting Information

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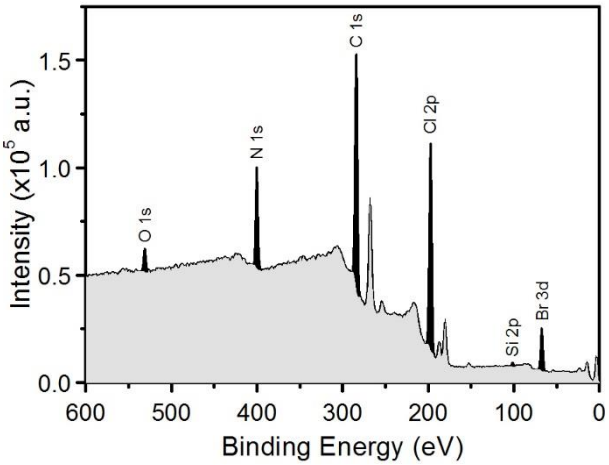


Figure S1. XPS survey scan of the amine-terminated Si NCs.

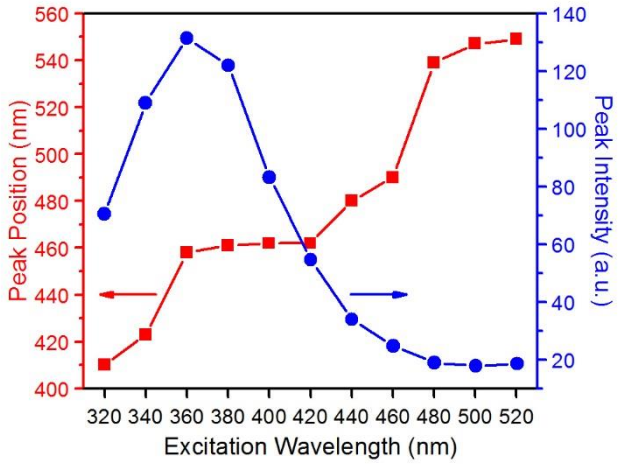


Figure S2. Luminescence peak position (red squares) and peak intensity (blue triangles) of the Si NCs versus excitation wavelength.

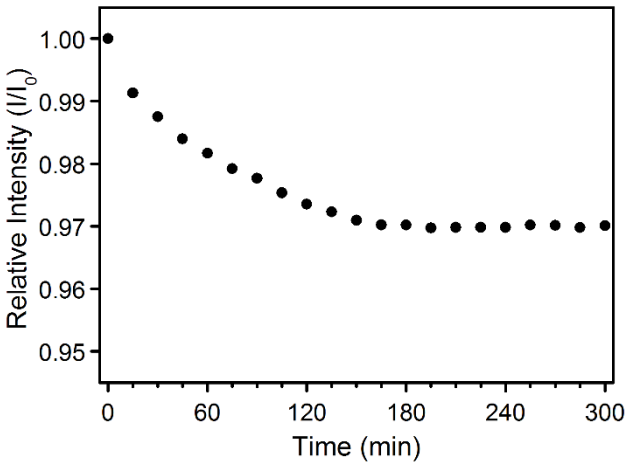


Figure S3. PL stability measurements (360 nm excitation) of the Si NCs recorded over 5 hours.

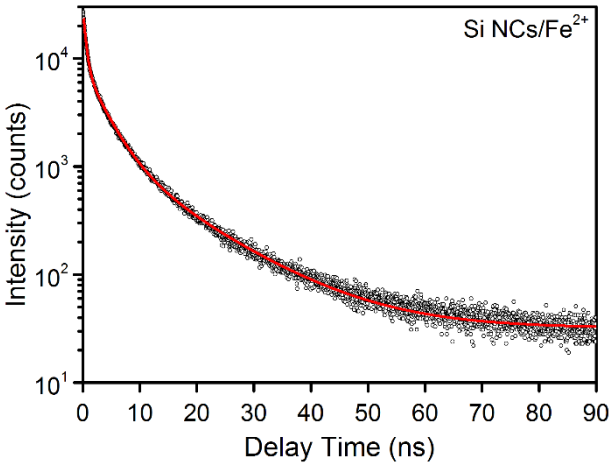


Figure S4. Nanosecond intensity transients of Si NCs in the presence of 50 μM Fe^{2+}.

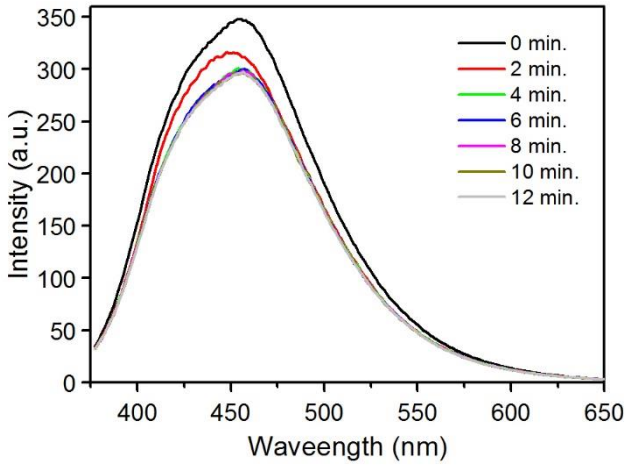


Figure S5. PL spectra of the Si NCs recorded before (0 min.) and after exposure to 50 μM Fe^{3+} for the times indicated.

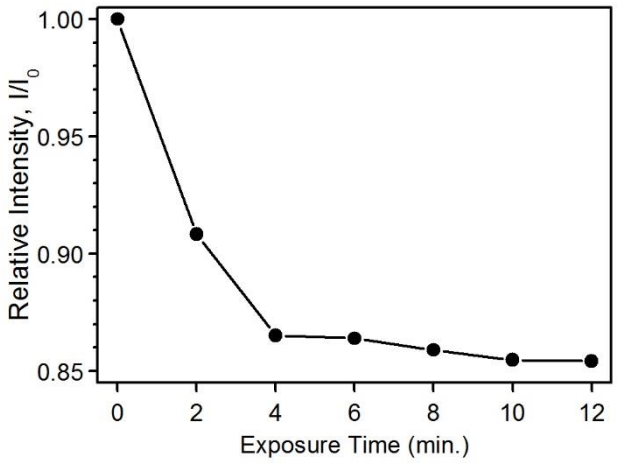


Figure S6. Relative integrated intensity of the Si NCs recorded before (0 min.) and after exposure to 50 μM Fe^{3+} for the times indicated.

Table S1. Fitted fractional amplitudes and time constants from three-component exponential fits to transients shown in Figures 6 and S4.

Sample	A_1	τ_1 [ns]	A_2	τ_2 [ns]	A_3	τ_3 [ns]	$\langle\tau\rangle_a$ [ns]	χ^2
Si NC	0.68	0.5	0.27	3.3	0.06	12.0	1.9	1.12
Si NC/Fe3+	0.70	0.4	0.25	3.1	0.06	11.6	1.8	1.04
Si NC/Fe2+	0.64	0.5	0.30	3.3	0.06	12.3	2.1	1.26

Table S2. Reduction potentials of selected metal ions.[1]

Reduction	E^0 [V *vs.* SHE]	Reduction	E^0 [V *vs.* SHE]
Mn^{2+}/Mn	-1.185	Cu^{2+}/Cu	0.3419
Fe^{3+}/Fe^{2+}	+0.771	Zn^{2+}/Zn	-0.7618
Fe^{2+}/Fe	-0.447	Cd^{2+}/Cd	-0.403
Co^{2+}/Co	-0.28	Hg^{2+}/Hg	+0.851
Ni^{2+}/Ni	-0.257	Pb^{2+}/Pb	-0.1262
Cu^{2+}/Cu^{+}	+0.153		

[1] from *Electrochemical Series*, P. Vanýsek, in *CRC Handbook of Chemistry and Physics*, 92th ed., (Ed: W.M. Haynes), CRC Press, Boca Raton, **2011**.

Calculation of the interaction region around the Nanocrystals

The volume of the spherical shell region surrounding the Si NCs is given by the difference of two spherical volumes, assuming the partial volume occupied by the allylamine ligands is neglected. **Scheme S1** shows a spherical Si NC of radius r_{NC}, surrounded by a sphere of radius $R = r_{NC} + d_{rms}$, where d_{rms} is the root-mean-square diffusion distance of the ferric ions during the luminescence lifetime.

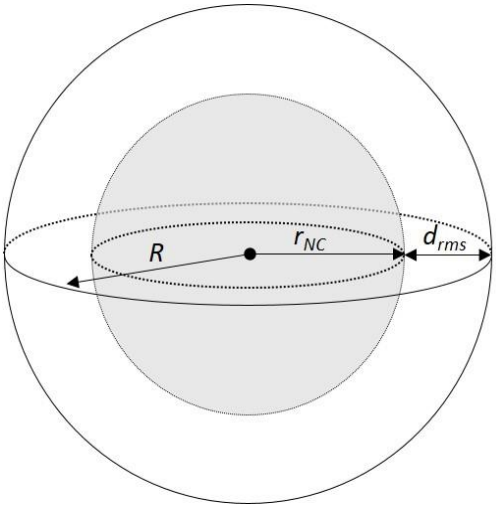
The difference in volume of the two spheres is given by:

$$V = \frac{4}{3}\pi R^3 - \frac{4}{3}\pi {r_{NC}}^3$$

which simplifies to:

$$V = \frac{4}{3}\pi (R^3 - {r_{NC}}^3)$$

For a Si NC with an average NC radius of 2.7 nm, and a ferric ion diffusion distance of 1.5 nm, the volume of the interaction region is 2.3 x 10^{-25} m^3.



Scheme S1. Schematic of a Si NC of radius r_{NC}, surrounded by a spherical shell of thickness d_{rms}.