Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information (ESI)

Switching-on Superparamagnetism in diluted magnetic Fe (III) doped CdSe Quantum Dots

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S.1 EDX analysis of Fe doped CdSe QDs

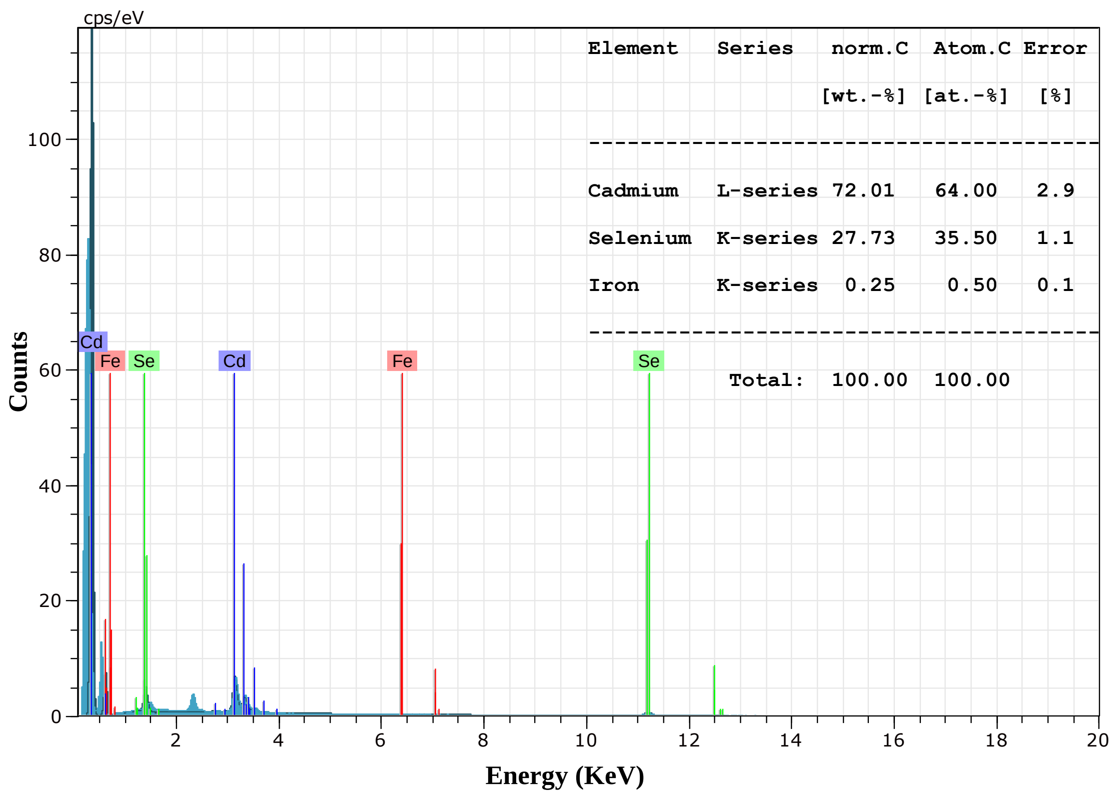


Figure S.1 EDX spectrum of Fe doped CdSe QDs. Inset shows elemental mapping of Fe doped CdSe QDs

S.2 TRPL Fitting

The PL decay curves of CdSe and Fe doped CdSe QDs can be well fitted with a bi-exponential function, using the following equation

$$Y(\tau) = \boldsymbol{a_1}\, \boldsymbol{e^{\frac{-\tau}{\tau_1}}} + \boldsymbol{a_2}\, \boldsymbol{e^{\frac{-\tau}{\tau_2}}}$$

The average lifetime calculated by

$$\boldsymbol{\tau_{ave}} = \frac{a_1\tau_1^2 + a_2\tau_2^2}{a_1\tau_1 + a_2\tau_2}$$

Where τ_1 and τ_2 are the first and second component of decay time, a_1 and a_2 are corresponding amplitudes (1).

S.3 Field-dependent magnetization Curve

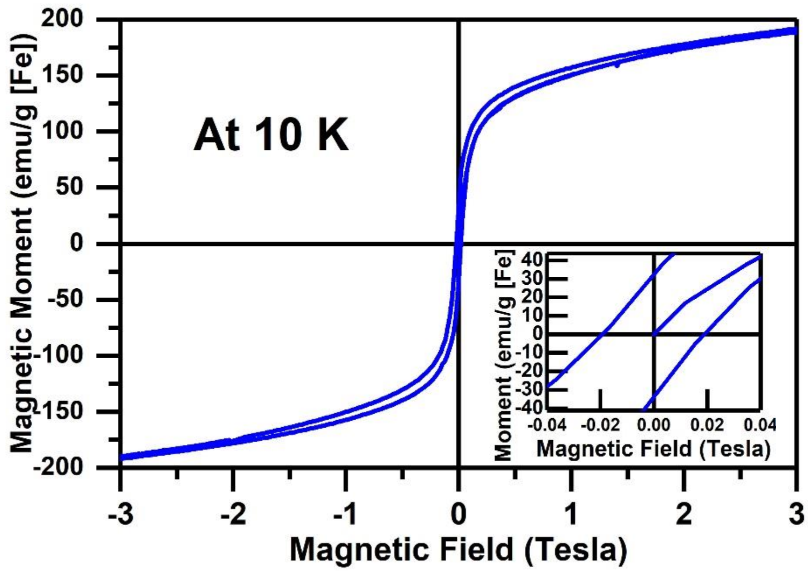


Figure S.2 MH curve for $Cd_{0.955}Fe_{0.005}Se$ QDs at 10 K. Inset image shows hysteresis loop.

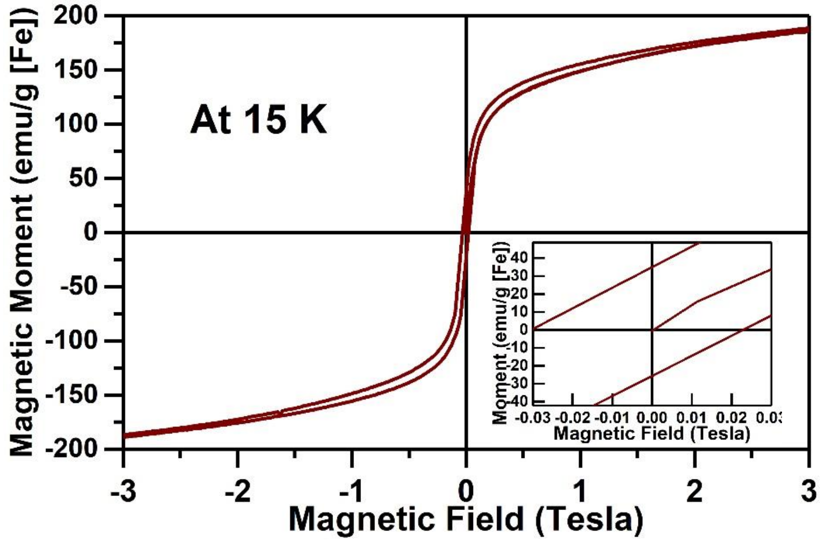


Figure S.3 MH curve of $Cd_{0.955}Fe_{0.005}Se$ QDs at 15 K. Inset image shows hysteresis loop.

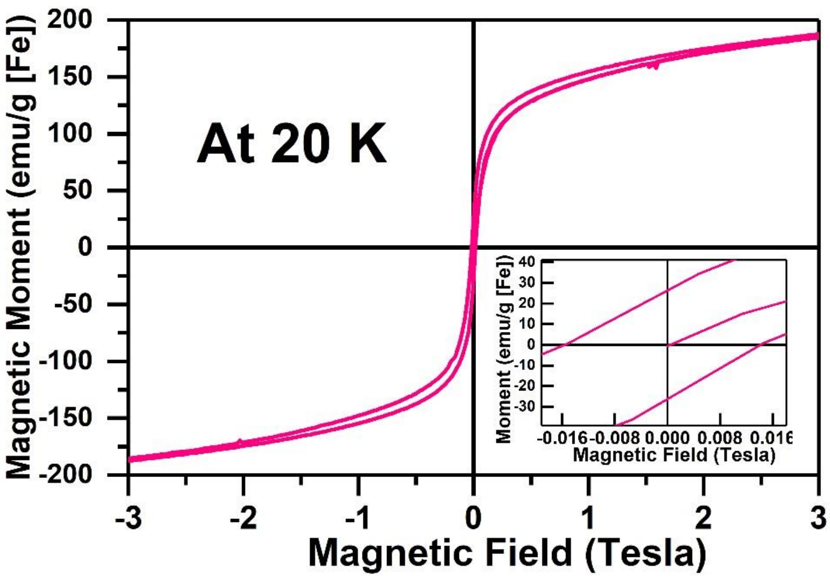


Figure S.4 MH curve of $Cd_{0.955}Fe_{0.005}Se$ QDs at 20 K. Inset image shows hysteresis loop.

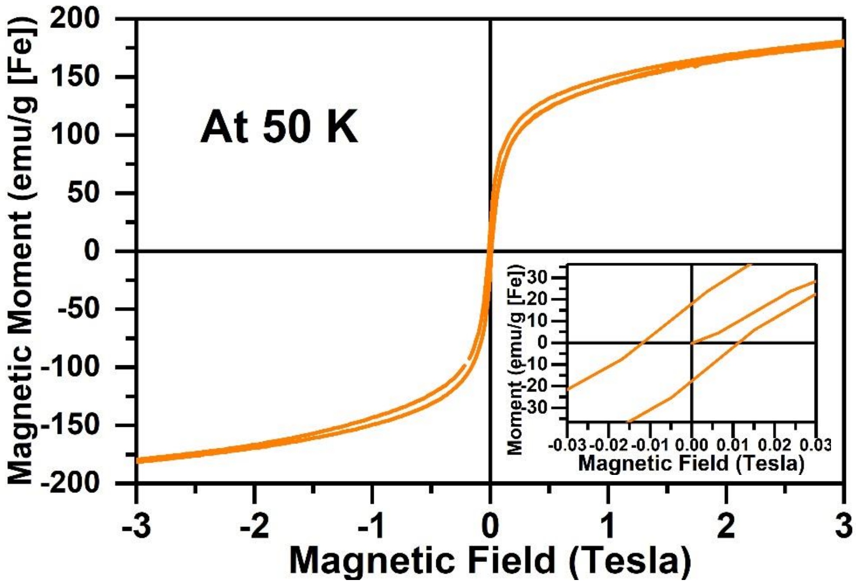


Figure S.5 MH curve of $Cd_{0.955}Fe_{0.005}Se$ QDs at 50 K. Inset image shows hysteresis loop.

Calculation of the number of atoms per QD lattice

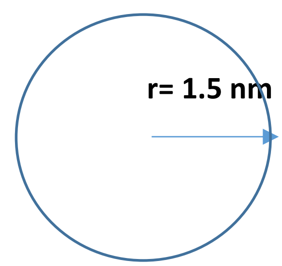
The calculation is as follows:

The volume of the sphere: $\frac{4}{3}\Pi r^3$

For 3 nm of Fe: CdSe QD, r = 1.5 nm

Thus, the volume of the QD, V_{QD} =14.13 nm^3

The volume of CdSe (wurtzite) unit cell, $V_{unit\ cell}$ = 0.112 nm^3



The number of the unit cells in 3 nm of Fe: CdSe QD

$$\mathbf{N = \frac{V_{QD}}{V_{unit\ cell}} \sim 126}$$

Since 1 unit cell of CdSe (wurtzite) has **4** atoms, hence we have 126*4= **504** number of total (**Cd and Se**) atoms.

Which means for 0.5% Fe doped CdSe QD, we have an average of ~ **2 Fe** atoms

References

1. A. N. Yadav, A.K. Singh, S. Srivastava, M. Kumar, B.K. Gupta, K. Singh, Phys. Chem. Chem. Phys., 2019, 21, 6265