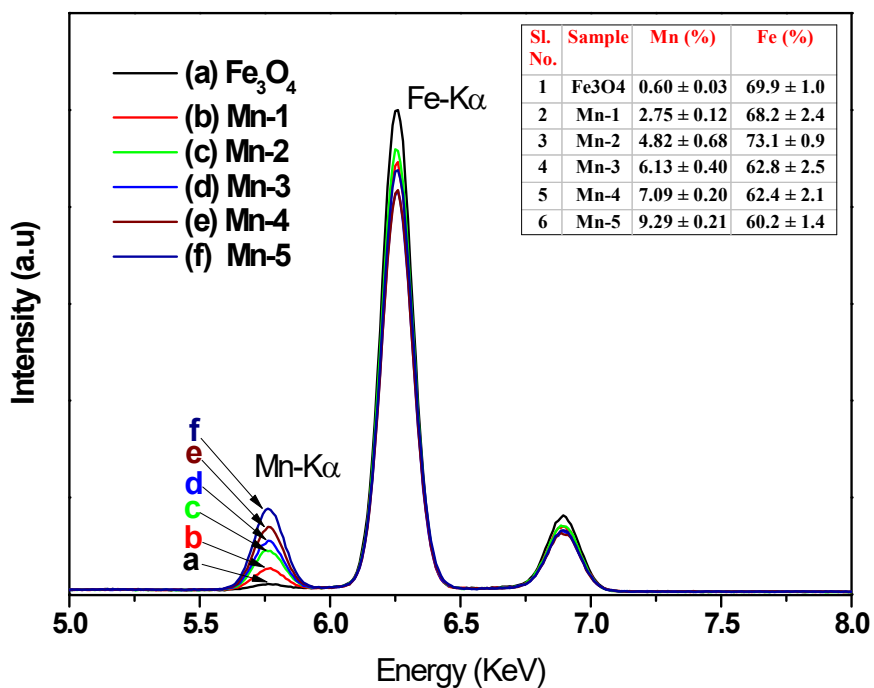## Supplementary Information

## A Rationale for Rapid Extraction of Ultra-low level Uranyl ion in Simulated Bioassays regulated by Mn-dopants over Magnetic Nano Particles

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| Sl. No. | Sample | Mn (%) | Fe (%) |
|---|---|---|---|
| 1 | Fe3O4 | 0.60 ± 0.03 | 69.9 ± 1.0 |
| 2 | Mn-1 | 2.75 ± 0.12 | 68.2 ± 2.4 |
| 3 | Mn-2 | 4.82 ± 0.68 | 73.1 ± 0.9 |
| 4 | Mn-3 | 6.13 ± 0.40 | 62.8 ± 2.5 |
| 5 | Mn-4 | 7.09 ± 0.20 | 62.4 ± 2.1 |
| 6 | Mn-5 | 9.29 ± 0.21 | 60.2 ± 1.4 |

**Fig.S-1**: ED-XRF data for the different Mn-doped $Fe_3O_4$ system; a) undoped $Fe_3O_4$; b) Mn-1 c) Mn-2 d) Mn-3 e) Mn-4 f) Mn-5

**Table S-1:** Atomic Weight Percentage of Elements as calculated from EDS data

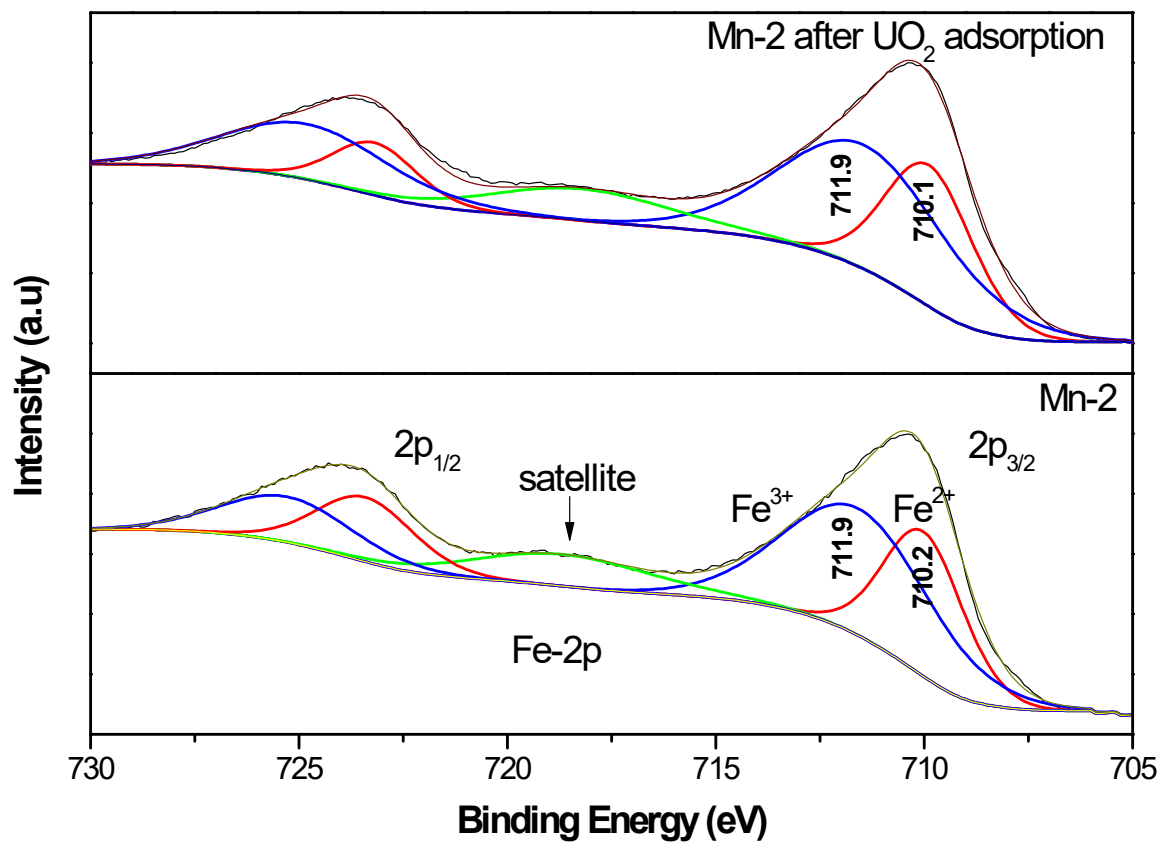| Sample | Fe | O | Mn |
|---|---|---|---|
| $Fe_3O_4$ | 32.7 | 67.3 | 0 |
| Mn-1 | 30.6 | 68.1 | 1.3 |
| Mn-2 | 29.7 | 67.8 | 2.5 |
| Mn | 27.6 | 67.7 | 4.7 |

**Fig. S-2:** XPS Spectra for Fe-2p for comparison of the process of sorption interaction; a) Mn-2 before uranyl sorption and b) Mn-2 after uranyl sorption post drying.
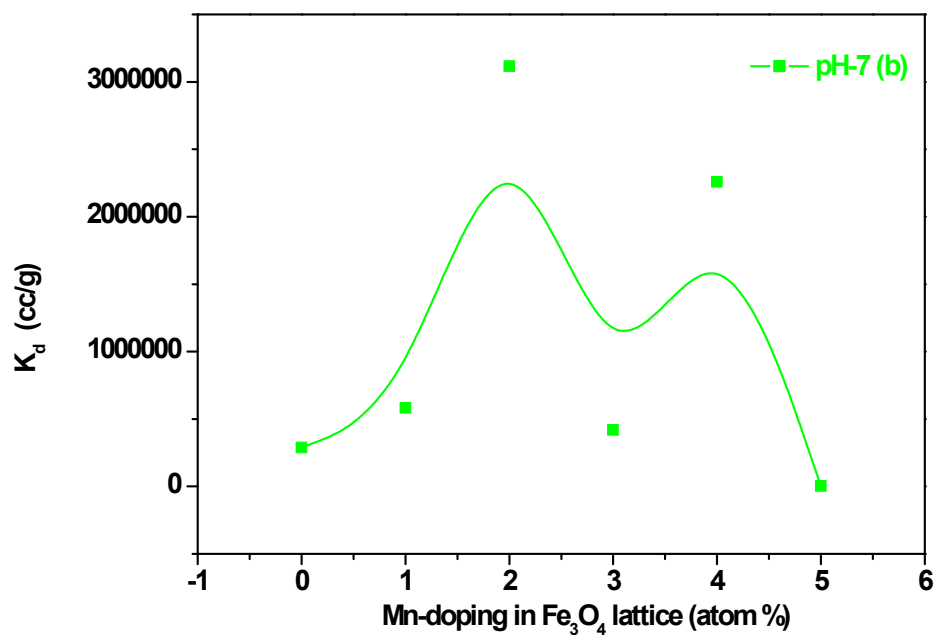


**Fig S-3:** Plot for $K_d$ versus the Mn-doping (atom %) in the $Fe_3O_4$ lattice at neutral medium (pH-7).

**Table S-2**: SAED calculation for $Fe_3O_4$ system.

| 1/D (nm$^{-1}$) | 1/r (nm$^{-1}$) | r (nm) | d-spacing (Å) | d-spacing (Å) (JCPDS-75-449) | h k l (JCPDS-75-449) |
|---|---|---|---|---|---|
| 6.893 | 3.4465 | 0.2901 | 2.9015 | 2.9380 | 2 2 0 |
| 8.08 | 4.04 | 0.2475 | 2.4752 | 2.5055 | 3 1 1 |
| 9.655 | 4.8275 | 0.2071 | 2.0715 | 2.0775 | 4 0 0 |
| 12.66 | 6.33 | 0.1580 | 1.5798 | 1.5992 | 5 1 1 |
| 13.645 | 6.8225 | 0.1466 | 1.4657 | 1.4690 | 4 4 0 |
| 18.671 | 9.3355 | 0.1071 | 1.0712 | 1.1104 | 6 4 2 |

**Table S-3**: SAED calculation for Mn dopped $Fe_3O_4$ system (Mn-3).

| 1/D (nm$^{-1}$) | 1/r (nm$^{-1}$) | r (nm) | d-spacing (Å) | d-spacing (Å) (JCPDS-75-449) | h k l (JCPDS-75-449) |
|---|---|---|---|---|---|
| 6.913 | 3.4565 | 0.2893 | 2.8931 | 2.9380 | 220 |
| 7.992 | 3.996 | 0.2502 | 2.5025 | 2.5055 | 311 |
| 9.664 | 4.832 | 0.2070 | 2.0695 | 2.0775 | 400 |
| 12.843 | 6.4215 | 0.1557 | 1.5573 | 1.5992 | 511 |
| 13.627 | 6.8135 | 0.1468 | 1.4677 | 1.4690 | 440 |

**Table- S-4**: Optimisation of the K-points for the bulk calculation of $Fe_3O_4$

| Sl. No. | K -Points | ΔE (eV)/atom | Magnetic Moment |
|---|---|---|---|
| 1 | 1 1 1 | -2.487617 | 59 |
| 2 | 3 3 3 | -2.577881 | 48 |
| 3 | 5 5 5 | -2.577813 | 48 |

**Table -S-5**: Comparison of Cell parameters for $Fe_3O_4$ and Mn-doped $Fe_3O_4$ system.

| Sl. No. | Mn-doping | Cell Parameter (a=b=c) (Å) Experimental | Cell Volume (Å)³ Experimental | Cell Parameter (a=b=c) (Å) Computational | Cell Parameter (a=b=c) (Å)³ Computational |
|---|---|---|---|---|---|
| 1 | 0 ($Fe_3O_4$) | 8.346(2) | 581.54(0.28) | 8.43036 | 599.15173 |
| 2 | Mn-1(Oct) | 8.369(4) | 586.24(0.51) | 8.43877 | 600.94877 |
| 3 | Mn-1(tet) | 8.369(4) | 586.24(0.51) | 8.34808 | 581.78137 |
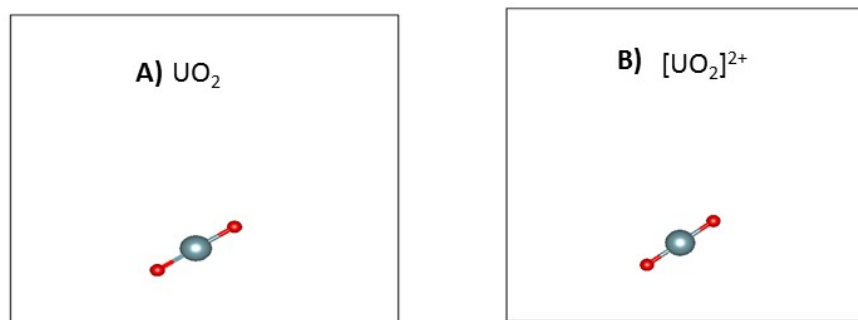


**Fig. S-4**: Optimised structures for A) $UO_2$ and B) $UO_2$-ion.

**Table -S-6**: Energy and bond Length for calculated UO2 and $[UO_2]^{2+}$- ion system.

| Sample | Energy (eV) | U-O (length) (Å) |
|---|---|---|
| $UO_2$ | -28.745974 | 1.8201 |
| $[UO_2]^{2+}$ | -12.759074 | 1.7284 |

## B. Calculation of Interaction Energy of $[UO_2]^{2+}$ ion with the Mn-doped Fe3O4 (3 1 1) Surface

Interaction Energy= Energy of $[UO_2]^{2+}$ adsorbed at particular site in Mn- doped $Fe_3O_4$ (3 1 1) surface - Slab energy Mn- doped $Fe_3O_4$ (3 1 1) surface

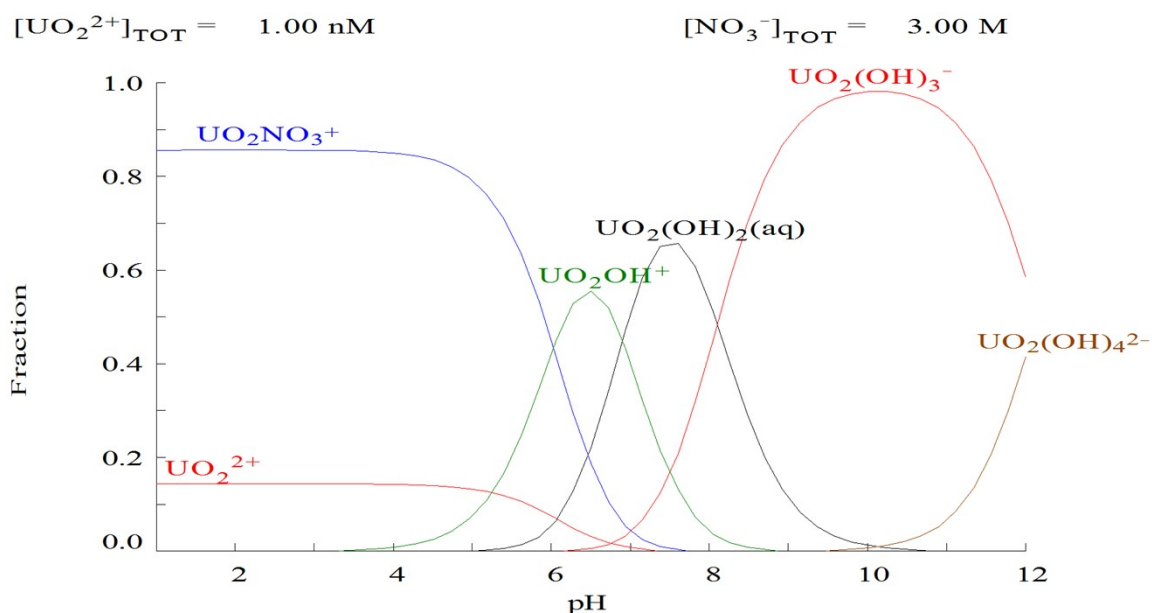- Energy of $[UO_2]^{2+}$ ion  .........(4)

Slab energy Mn-doped $Fe_3O_4 =$ -824.80301eV

Energy of $[UO_2]^{2+}$ ion $=$ -12.759074eV

Interaction energy with $Mn^{2+}$ site $=$ -854.61019 + [824.80301+12.759074] eV

$$= -17.048144 \text{ eV}$$

Interaction Energy with Fe-Tetrahedral ($Fe^{3+}$) site $=$ - 853.83122 +

$$[824.80301+12.759074] \text{ eV}$$

$$= -16.269136 \text{ eV}$$

Interaction energy with Fe-Octahedral ($Fe^{2+}$) site $=$ - 853.85384 +

$$[824.80301+12.759074] \text{ eV}$$

$$= - 16.29179 \text{ eV}$$



**Fig.S-5**: Speciation of Uranyl ion at different pH (Concentration of $UO_2^{2+}$= 1nM and $NO_3^-$ = 3M) as suggested in the experimental section. The Figure is made by the MEDUSSA HYDRA- Software plot.