Electronic Supplementary Material (ESI) for Environmental Science: Nano.

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Magnetic In-Pd Catalysts for Nitrate Degradation

Sujin Guo[1,2], *Camilah D. Powell*[2,3], *Dino Villagran*[2,4] *and Michael S. Wong*[1,2,3,5,6]*

[1]Department of Civil & Environmental Engineering, Rice University, 6100 Main Street, Houston, TX 77005, [2]Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment, [3]Department of Chemical and Biomolecular Engineering, Rice University, 6100 Main Street, Houston, TX 77005, [4]Department of Chemistry and Biochemistry, University of Texas at El Paso, El Paso, TX 79968, [5]Department of Chemistry, Rice University, 6100 Main Street, Houston, TX 77005, [6]Department of Materials Science and NanoEngineering, Rice University, 6100 Main Street, Houston, TX 77005

***To Whom Correspondence Should Be Addressed** E-mail: mswong@rice.edu

Table S1 NEWT general test water (fresh) – for drinking water

General Paramaters	*Specification*	
Water Source	De-ionized water (conductivity < 1 μ S/cm)	
pH adjusted with HCl	7.5±0.25	
Temperature	20±2.5 ℃	
Constituents	*Concentration (mg/L)*	*Concentration (mM)*
Bicarbonate (HCO_3^-)	183	3.0
Chloride (Cl^-)	71	2.0
Sulfate (SO_4^{2-})	48	0.50
Silicate (SiO_2^{2-})	21.4	0.33
Nitrate (NO_3^-)	8.9 (2.0 as N)	0.14
Phosphate (PO_4^{3-})	0.12 (0.04 as P)	0.0013
Fluoride (F^-)	1.0	0.053
Calcium (Ca^{2+})	40	1.0
Magnesium (Mg^{2+})	12	0.50
Sodium (Na^+)	89	3.86
Total dissolved solids (TDS)	478	-
Ionic strength	-	8.5

Table S2 Magnetic properties of nFe_3O_4, $nFe_3O_4@SiO_2$ and Pd-In/$nFe_3O_4@SiO_2$

Compound	*Magnetic Saturation Ms (emu/g)*	*Magnetic Remanence Mr (emu/g)*	*Magnetic Remanance/Magnetic Saturation*	*Coercivity (kOe)*
nFe_3O_4	77.1	7.0	0.091	0.06
$nFe_3O_4@SiO_2$	56.0	4.5	0.080	0.07
Pd-In/$nFe_3O_4@SiO_2$	29.5	2.5	0.085	0.18

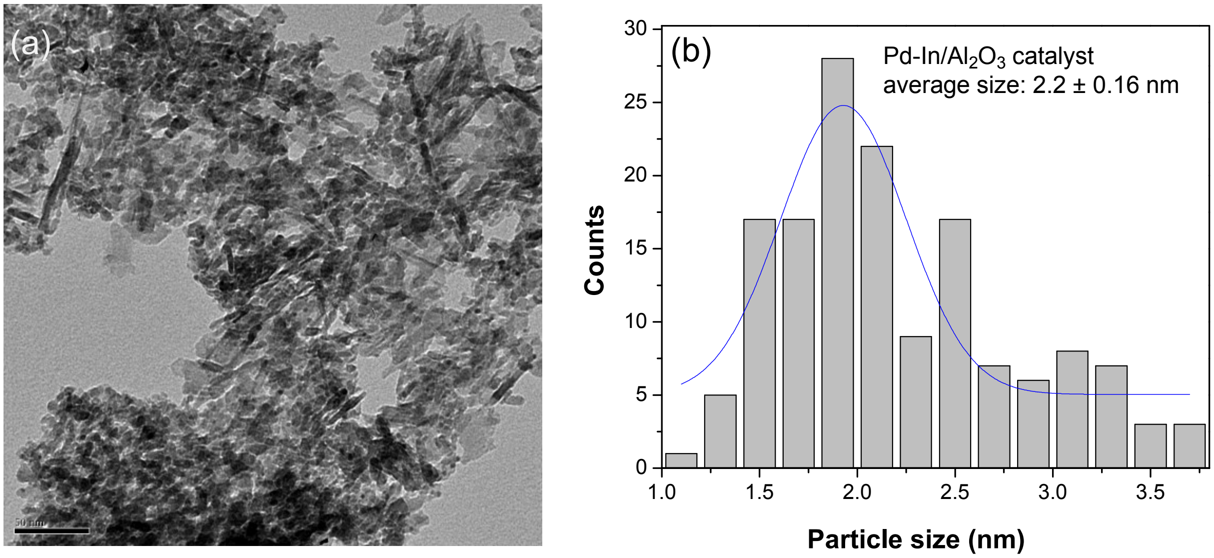

Fig. S1 (a) TEM image of Pd-In/Al_2O_3 catalyst (scale bar = 50 nm) and (b) Pd particle size distribution the Pd-In/Al_2O_3 catalyst

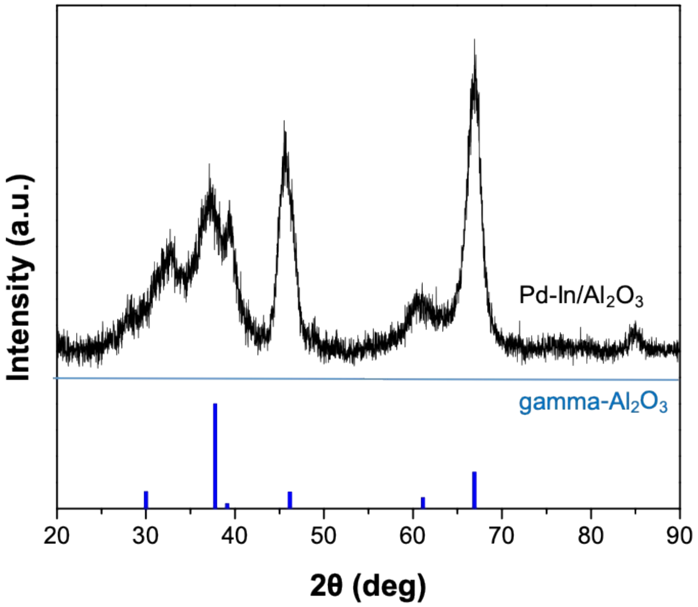

Fig. S2 XRD spectrum of Pd-In/Al_2O_3 sample.

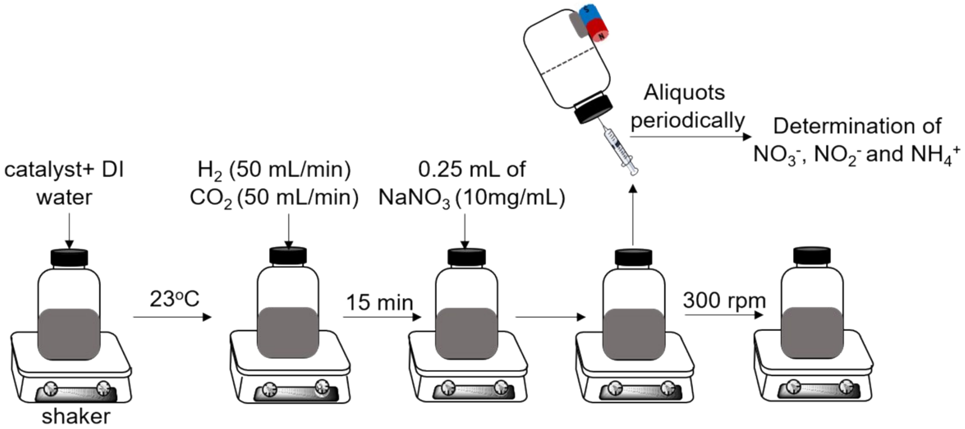

Fig. S3 Schematic of the experimental setup

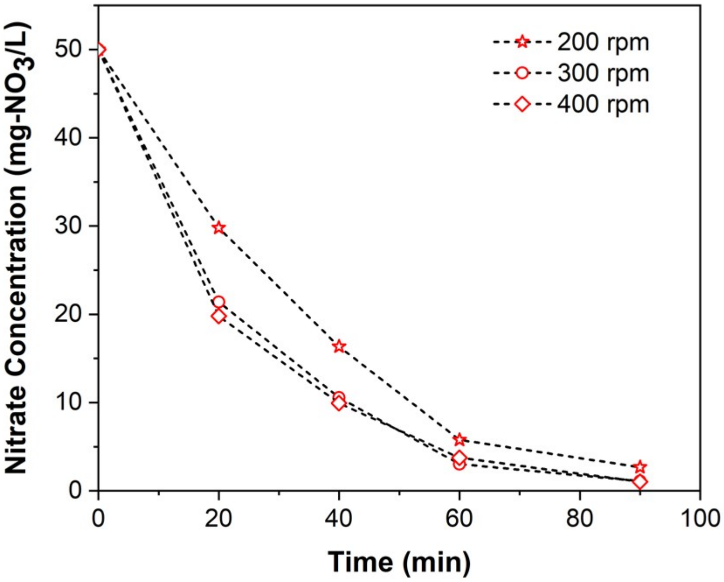

Fig. S4 Changing shaking speed to check the external mass transfer. Reaction conditions: 1 g/L catalyst loading, 200, 300 and 400 rpm string rate, 1 atm pressure, DI water containing nitrate.

The Weisz–Prater parameter (C_{WP}) was used to evaluate internal mass transfer limitations, as described in the following formula:

$$C_{WP} = \frac{R^2 k_{obs} \tau}{D\theta}$$

where k_{obs} is the observed pseudo-first-order rate constant for nitrate reduction (0.0616 s^{-1}) from Fig. 3, R is the catalyst's radius, τ is the tortuosity factor of the catalyst (typically varies from 2 to 10), θ is the porosity of the catalyst (typically varies from 0.2 to 0.7), and D is the diffusion coefficient of nitrate in water (1.7×10^{-8} m^2 s^{-1}). The reaction is significantly limited by internal mass transfer while C_{WP} is much greater than 1, while is negligible when C_{WP} is much less than 1. If we choose the smallest θ value (0.2), largest τ value (10) and R value (1 μm) to estimate the maximum value of C_{WP}. The calculated maximum C_{WP} was 3.6×10^{-6}, much less than 1. Thus, internal mass transfer limitations are also negligible for our Pd-In/Fe_3O_4 catalyst in the nitrate reduction. For the SiO_2 coated catalyst, the surface radius is supposed to be larger than Pd-In/Fe_3O_4 and θ will be smaller, while the estimated C_{WP} was still smaller than 1.

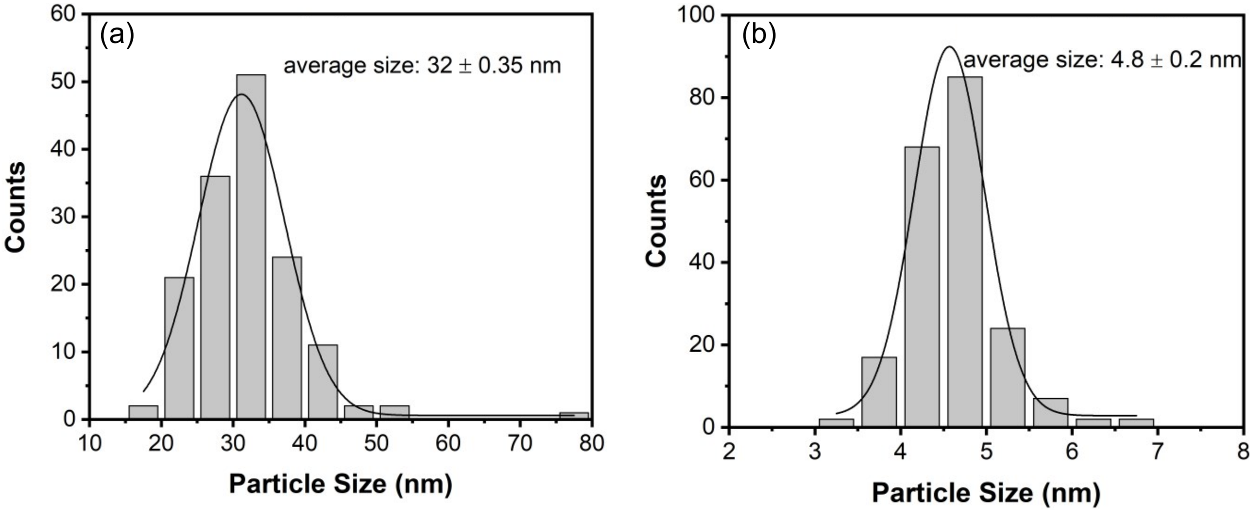

Fig. S5 Particle size distribution of (a) nFe_3O_4 and (b) Pd-In NPs of Pd-In/nFe_3O_4@SiO_2 catalyst material.

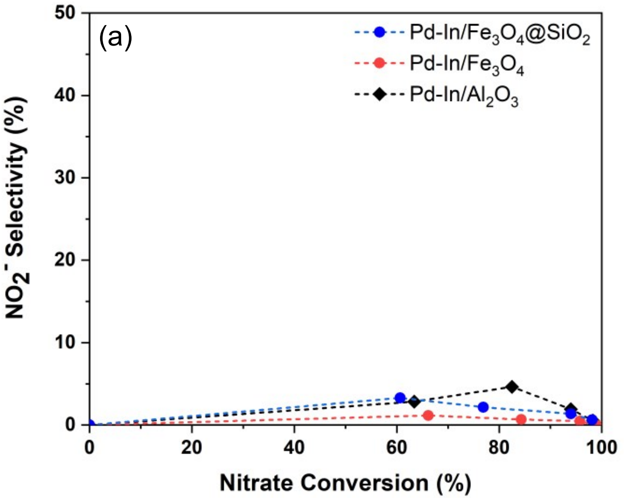

Fig. S6 Selectivity of the Pd-In/nFe$_3$O$_4$@SiO$_2$, Pd-In/nFe$_3$O$_4$ and Pd-In/Al$_2$O$_3$ catalysts to nitrite and ammonium as a function of nitrate conversion in DI water. (a) S NO$_2$- , (b) S NH$_4^+$. Reaction conditions: 1 g/L catalyst loading, 300 rpm string rate, 1 atm pressure, DI water containing nitrate.

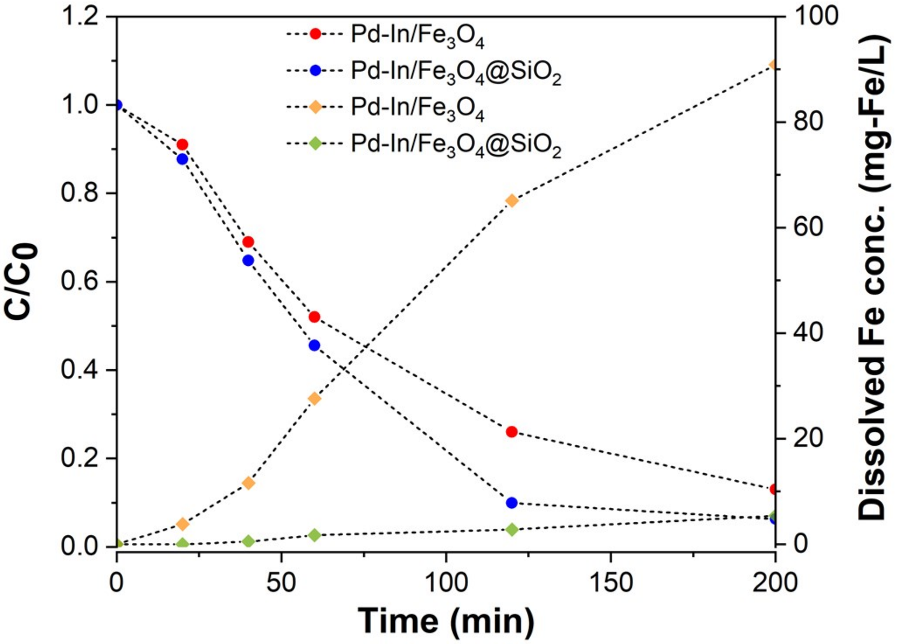

Fig. S7 Nitrate reduction kinetics in SDW for Pd-In/nFe$_3$O$_4$ (red) and Pd-In/nFe$_3$O$_4$@SiO$_2$ (blue), and the corresponding iron leaching concentration during the first cycle. Reaction conditions: 1 g/L catalyst loading, 300 rpm string rate, 1 atm pressure, SDW containing nitrate (~50 ppm).

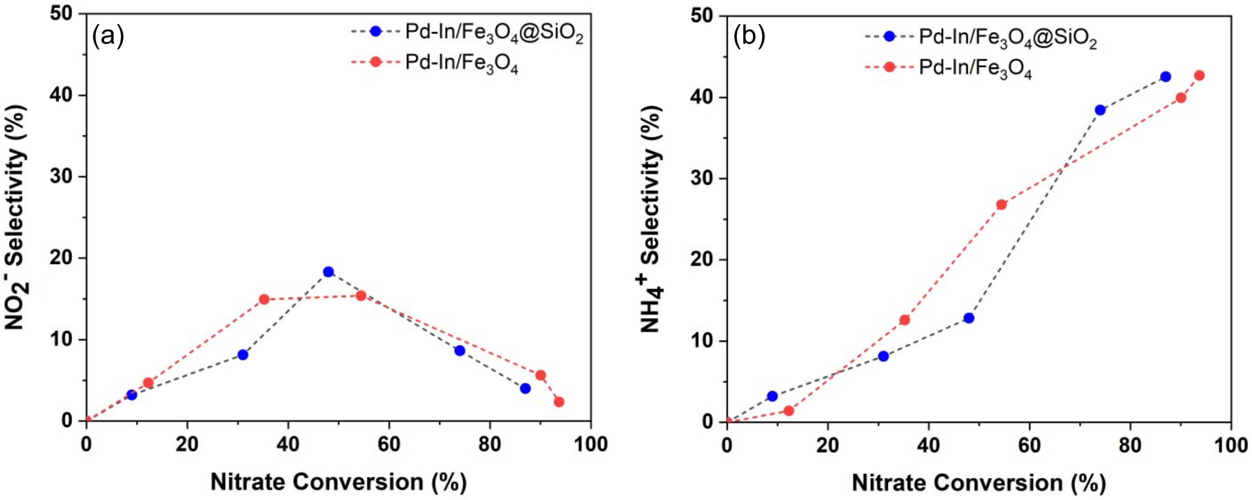

Fig. S8 Selectivity of the Pd-In/nFe$_3$O$_4$@SiO$_2$ and Pd-In/nFe$_3$O$_4$ catalysts to nitrite and ammonium as a function of nitrate conversion in SDW. (a) S NO$_2$-, (b) S NH$_4^+$. Reaction conditions: 1 g/L catalyst loading, 300 rpm string rate, 1 atm pressure, DI water containing nitrate.