Supplementary Information

FePd nanowires modified with cyclodextrin as improved catalysts: Effect of the alloy composition on colloidal stability and catalytic.

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1. Energy Dispersive X-Ray Spectroscopy.

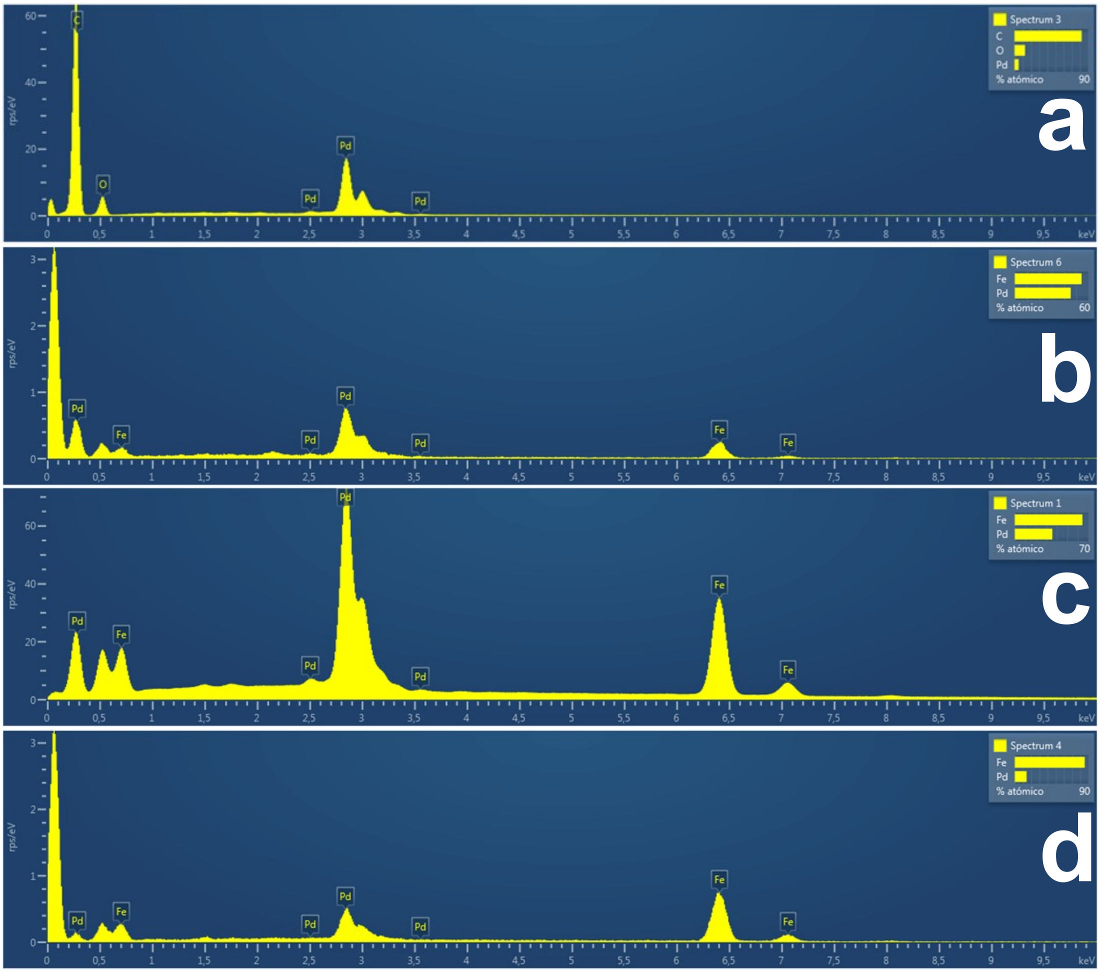

Figure S1.EDS spectra for FePd NWs of different composition. a) Pd b) $Fe_{55}Pd_{45}$ c) $Fe_{65}Pd_{35}$ d) and e) $Fe_{85}Pd_{15}$.

Table S1. Atomic % composition, calculated from XPS data.

Element	Atomic%	Atomic%[a]
C	15.9	
Pd	30.0	35.6
Fe	54.1	64.4

[a] atomic % recalculated without considering C.

2. UV.vis measurements

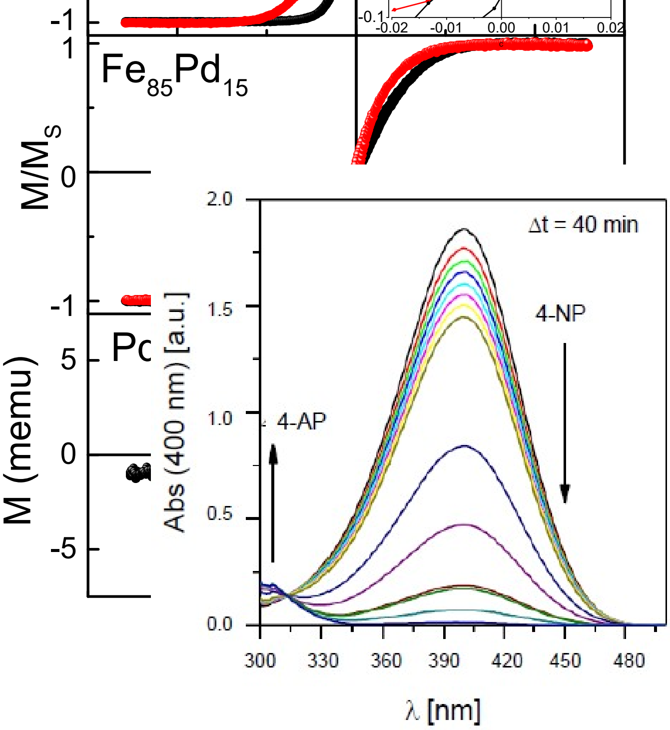

Figure S2. UV-vis spectra at different times of the reduction reaction of 4-NP 10^{-4} M in aqueous solution containing $NaBH_4$ 0.1 M and FePd NWs@βCDMOD14

3. Catalytic studies

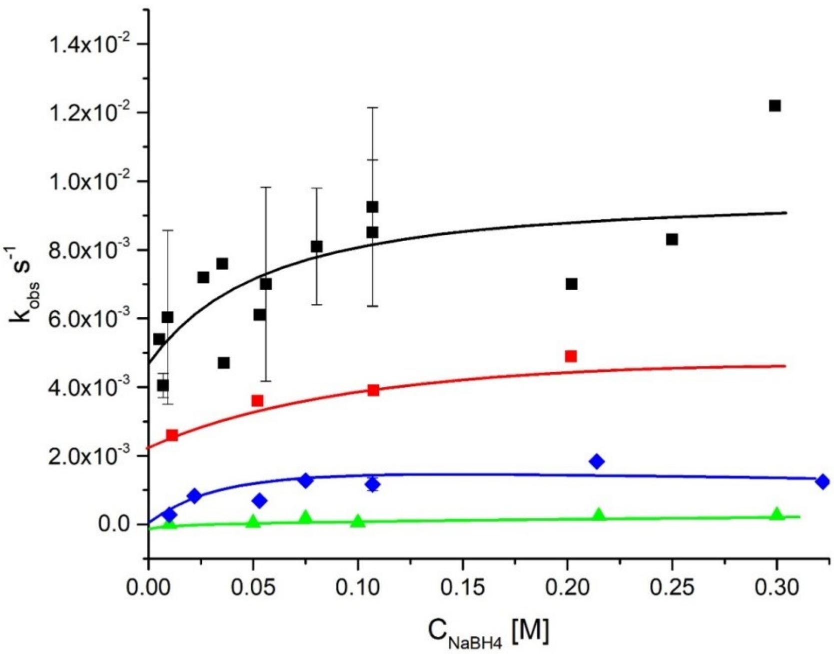

Figure S3. k_{obs} vs $[NaBH_4]$ for reaction of 4-NP in presence of different alloys FePdNW@βCDMOD14. $Fe_{55}Pd_{45}$ (black line), $Fe_{65}Pd_{35}$ (red line), Pd (blue line) and $Fe_{85}Pd_{15}$ (green line).

$$\theta_{4-NP} = \frac{\left(K_{4-NP}[4-NP]\right)^n}{1+\left(K_{4-NP}[4-NP]\right)^n + \left(K_{BH_4^-}[BH_4^-]\right)^n} \quad \text{Eq.S1}$$

$$\theta_{BH_4^-} = \frac{\left(K_{BH_4^-}[BH_4^-]\right)^n}{1+\left(K_{4-NP}[4-NP]\right)^n + \left(K_{BH_4^-}[BH_4^-]\right)^n} \quad \text{Eq.S2}$$

3.a. The Taylor series expansion

The deduction of formula (Eq. 6) is as follows: According Eq. 5, we consider that kobs is a function of [4-NP] variable and descripted by a rational function, $\frac{f}{g}$, Eq.S3:

$$k_{obs} = \frac{f}{g} = \frac{kSK_{4-NP}K_{BH_4^-}\left[BH_4^-\right]}{\left(1+K_{4-NP}\left[4-NP\right]+K_{BH_4^-}\left[BH_4^-\right]\right)^2} \quad \text{Eq.S3}$$

Where f and g are descripted by Eq. S4 and Eq.S5 respectively,

$$f = \left(kSK_{4-NP}K_{BH_4^-}\left[BH_4^-\right]\right) \quad \text{Eq.S4}$$

$$g = \left(1+K_{4-NP}\left[4-NP\right]+K_{BH_4^-}\left[BH_4^-\right]\right)^2 \quad \text{Eq.S5}$$

We use the Taylor expansion around [4-NP]=0 to obtain a linear approximation of Eq.S3 by truncating at the first-order (Eq. S6)

$$k_{obs} \approx k_{obs}\left(0\right)+\frac{\partial k_{obs}}{\partial[4-NP]}\left(0\right).[4-NP] \quad \text{Eq. S6}$$

Where the first derivate ($\frac{\partial k_{obs}}{\partial[4-NP]}$) was obtained through the derivatives of rational function and according to the following rule (Eq.S7):

$$\frac{\partial k_{obs}}{\partial[4-NP]} = \frac{f'.g-f.g'}{g^2} \quad \text{Eq.S7}$$

Where f' and g' are the derivates of f and g respectively and descripted by Eq. S8 and Eq. S9

$$f' = 0 \quad \text{Eq. S8}$$

$$g' = 2.K_{4-NP}.\left(1+K_{4-NP}\left[4-NP\right]+K_{BH_4^-}\left[BH_4^-\right]\right) \quad \text{Eq. S9}$$

If we substitute Eq. S4, S5, S8 and S9 into Eq. (S7) evaluated at [4-NP]=0, we obtained the slope of the linear approximation of Eq. S6 which is descripted by Eq. S10

$$\frac{\partial k_{obs}}{\partial[4-NP]}\left(0\right) = \frac{-2.k.S.\left(K_{4-NP}\right)^2.\left(K_{BH_4^-}\left[BH_4^-\right]\right)}{\left(1+\left(K_{BH_4^-}\left[BH_4^-\right]\right)\right)^3} = slope \quad \text{Eq.S10}$$

3.b. Determination of S.

The theoretical value of *S* (the total surface area of FePdNWs normalized to the solution's unit volume) was determined through the following equations. Geometrical parameters of cylindrical NWs (length and diameter), were obtained experimentally (see Table S1).

$$S_{NW} = 2\pi r h + 2\pi r^2 \qquad V_{NW} = \pi r^2 h$$

$$\rho_{Pd^\circ} = 12.02 \cdot 10^3 \frac{kg}{m^3} \qquad \rho_{Fe^\circ} = 7.85 \cdot 10^3 \frac{kg}{m^3}$$

PM_{Pd° = 106.42 g/molPM_{Fe° = 55.84 g/mol

Where r=100nm is the NW radius, and L is their length (values in table S1), V_{NW} and S_{NW} are the volume and the surface of each individual NW, respectively, ρPd and ρFe are the density of Pd^0 and Fe^0 , respectively, PM Pd^0 and PM Fe^0 are the molar mass of Pd^0 and Fe^0 , respectively.

The density of each FePdNW composition ($\rho Fe_{(100-x)}Pd_x$), the individual mass (mNW), the total quantity (N), the individual surface (SNW) and the surface in ´catalyst solution´ (S´cs´) were calculated by using the follow equation and values obtained informed in Table S1.

$$\rho_{Fe_{(100-x)}Pd_x} = \frac{[\rho_{Fe} \cdot (100-x)] + [\rho_{Pd} \cdot x]}{100}$$

$$m_{NW} = \rho_{Fe_{(100-x)}Pd_x} . V_{NW}$$

(see Sec. 2.2)

$S_{'cs'}$=N . S_{NW}/2.10^{-3}L

$$N = m_{NW} / m_{sample}$$

$$S_{'cs'} = S_{NW} / 2 \cdot 10^{-3}$$

Finally, S is the total surface which takes in account the dilution factor (50µL of NWs in 2.8mL)

Table S2: Geometrical parameters and constants for the different NWs alloys

Composition at%.	Length L^a [±2 µm]	$V_{NW}.10^{-20}$ m^3	ρ̇.10^3 kg/m^3	$m_{NW}.10^{-12}$ g	m mg	N.10^8	$S_{NW}.10^{-12}$ m^2	S.10^{-3} $m^2.L^{-1}$
$Fe_{85}Pd_{15}$	8	25.1	7.85	1.97	1.0±0.1	5.1	5.1	21
$Fe_{65}Pd_{35}$	22	69.1	9.31	6.43	0.4±0.1	0.6	13.9	7
$Fe_{55}Pd_{45}$	13	40.8	9.73	3.97	0.8±0.1	2.0	8.2	14

Fe_0Pd_{100}	10	31.4	12.02	3.78	0.5±0.1	1.3	6.3	7