

Supplementary information

Towards molecular batteries: coverage of small amino-silica nanoparticles with ferrocenyl and pentamethylferrocenyl groups and their redox properties.

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General data

For general data, see ref. 7a-c. The CVs were recorded at 25°C on a PAR 273 potentiostat galvanostat with Pt working and counter electrodes and Ag reference electrode. The E_{1/2} values were measured using decamethylferrocene as internal reference (see Figure SI-1). Infrared spectra were recorded on a FT-IR Paragon 1000 Perkin-Elmer spectrometer using neat samples in KBR disks.

Determination of the number of Fc groups per SiO₂ NP

Volume of a 12-nm SiO₂ NP core: $\frac{4}{3} \pi r^3 = 1.33 \times 3.14 \times (6 \cdot 10^{-7} \text{ cm})^3 = 0.756 \cdot 10^{-18} \text{ cm}^3$

Core mass = $0.756 \cdot 10^{-18} \times 2.2 = 1.66 \cdot 10^{-18} \text{ g}$

Additional mass of the 300 FcCONHC₃H₆SiO₂ chains: $0.2 \cdot 10^{-18} \text{ g}$

Total mass: $1.86 \cdot 10^{-18} \text{ g}$

Titration of a sample of 0.328 g of Fc SiO₂ NPs by 1.3 mL of FcCOMe⁺ (74 mM)

Number of Fc SiO₂ NPs in the sample: $0.328 / 1.86 \cdot 10^{-18} = 1.77 \cdot 10^{17}$

Number of moles of electrons exchanged at the equivalent point: $1.3 \cdot 10^{-3} \text{ L} \times 74 \cdot 10^{-3} \text{ mol/L} = 0.962 \cdot 10^{-4} \text{ mol}$

Number of electrons exchanged at the equivalent point = $0.962 \cdot 10^{-4} \text{ mol} \times 6.023 \cdot 10^{23} = 5.96 \cdot 10^{19}$ electrons (one electron *per* Fc group)

Number of electrons exchanged *per* Fc SiO₂ NP = $5.96 \cdot 10^{19} / 1.77 \cdot 10^{17} = 335$

Estimated error (end point) approx. 15%: **335 ± 50**

Determination of the number of Fc* groups per SiO₂ NP

Titration of a sample of 0.086 g of Fc* SiO₂ NPs by 1.0 mL of oxidant (18.7 mM)

Number of Fc SiO₂ NPs in the sample: $0.086 / 1.86 \cdot 10^{-18} = 0.47 \cdot 10^{17}$

Number of moles of electrons exchanged at the equivalent point: $1 \cdot 10^{-3} \text{ L} \times 18.7 \cdot 10^{-3} \text{ mol/L} = 1.87 \cdot 10^{-5} \text{ mol}$

Number of electrons exchanged at the equivalent point = $1.87 \cdot 10^{-5} \text{ mol} \times 6.023 \cdot 10^{23} = 1.12 \cdot 10^{19}$ electrons (one electron *per* Fc group)

Number of electrons exchanged *per* Fc SiO₂ NP = $1.12 \cdot 10^{19} / 0.47 \cdot 10^{17} = 240$

Estimated erreur (end point) approx. 15%: **240 ± 40**

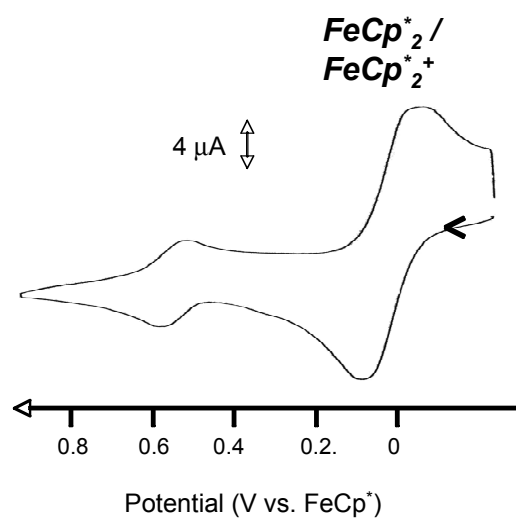


Figure 1. CV of $\text{Me}_3\text{Fc-SiO}_2$ NPs. Conditions are as follows: methanol 2 ml + CH_3CN 2 ml, working electrode: ITO, counter: Pt, Reference: Ag, 35 mg of the sample, 10 mM $n\text{-Bu}_4\text{N}^+\text{PF}_6^-$, 200 mV/s.

Figure SI-1. Cyclic voltammogram of $\text{Fc}^* \text{SiO}_2$ NPs in the presence of decamethylferrocene (PAR 273 potentiostat galvanostat)

