Electronic Supplementary Information (ESI)

Ligand-induced Reduction Concerted with Coating by Atomic Layer Deposition on the example of TiO_2-Coated Magnetite Nanoparticles

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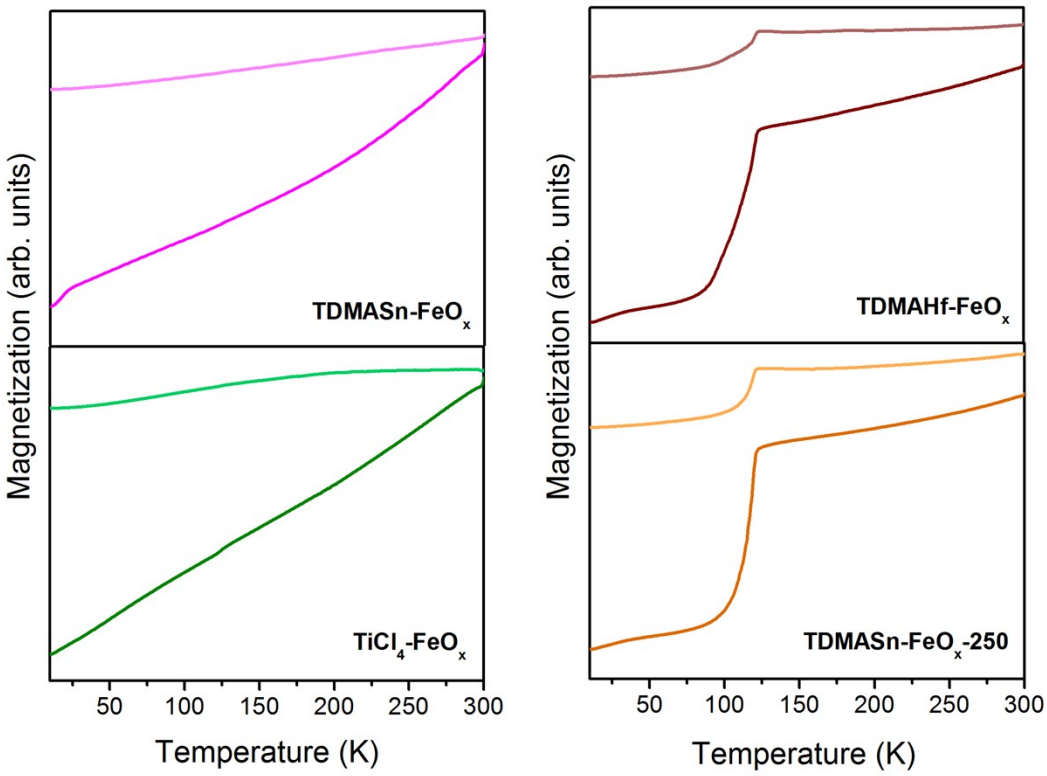

Figure S1. Magnetization vs. temperature of TiO_2-coated γ-Fe_2O_3 nanoparticles applying $TiCl_4$ and H_2O as ALD precursors ($TiCl_4$-FeO_x), SnO_2-coated γ-Fe_2O_3 nanoparticles with TDMASn and H_2O as ALD precursors, at 150ºC (TDMASn-FeO_x) and at 250 ºC (TDMASn-FeO_x-250) process temperatures and HfO_2-coated γ-Fe_2O_3 nanoparticles with TDMAHf and H_2O ALD precursors (TDMAHf-FeO_x).

Table S1. List of possible reaction schemes and DFT calculated reaction energies for reducing Fe_2O_3 to Fe_3O_4 by using different ALD precursors.

Precursor	Electronegativity	Reaction products	Activation barrier (eV)
TDMAHf	1.3	HfO_2, $(CH_3)_2NN(CH_3)_2$	-0.37
TDMAZr	1.33	ZrO_2, $(CH_3)_2NN(CH_3)_2$	-0.25
TDMATi	1.54	TiO_2, $(CH_3)_2NN(CH_3)_2$	0.85
TDMASn	1.96	SnO_2, $(CH_3)_2NN(CH_3)_2$	1.12
TDMAIr	2.20	IrO_2, $(CH_3)_2NN(CH_3)_2$	2.16
$Ti(OiPr)_4$	1.54	TiO_2, $(CH_3)_2O$, $(CH_3)_2OH$	4.08
$TiCl_4$	1.54	TiO_2, Cl_2	4.45

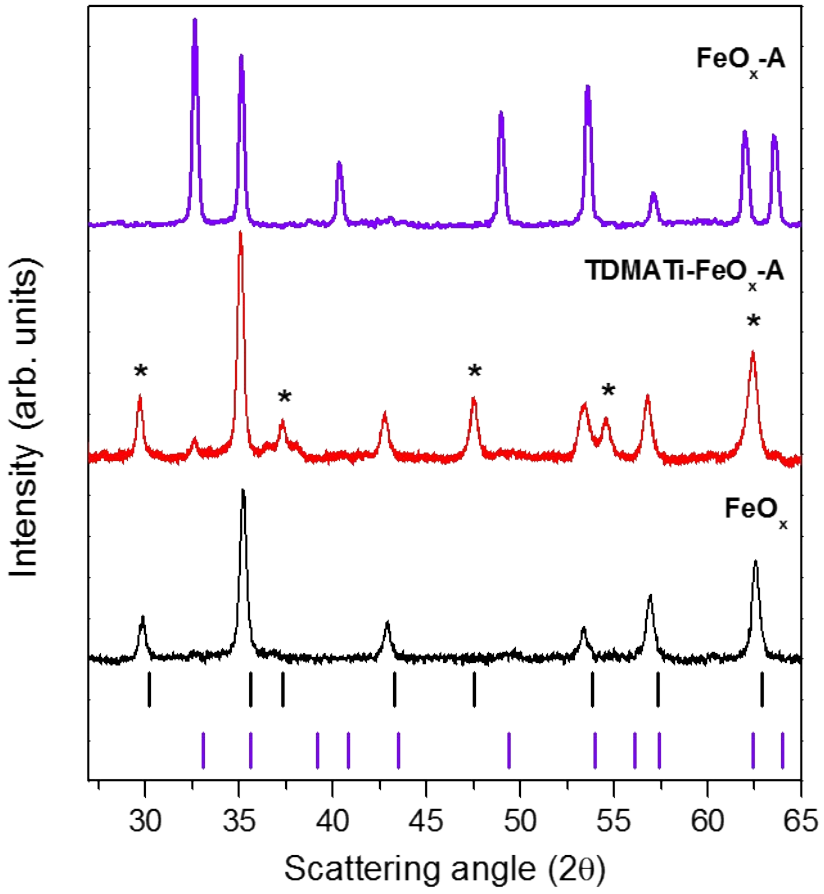

Figure S2. XRD patterns of γ-Fe_2O_3 nanoparticles (FeO_x), TiO_2-coated γ-Fe_2O_3 nanoparticles with TDMATi and H_2O as precursors, after annealing at 470ºC (TDMATi-FeO_x-A) and uncoated γ-Fe_2O_3 nanoparticles after annealing at 470ºC (FeO_x-A). The bars at the bottom show the theoretical peak position of the γ-Fe_2O_3/Fe_3O_4 (black) and α-Fe_2O_3 (violet) crystallographic phases.