Supporting information for

Nanostructured Co_xNi_{1-x} bimetallic alloys for high efficient and ultrafast adsorption: experiments and first-principles calculations

Haiming Sun, Xijia Yang, Lijun Zhao*, Yue Li, Jiamu Zhang, Lu Tang, Yining Zou, Cong Dong, Jianshe Lian* and Qing Jiang

Key Laboratory of Automobile Materials (Jilin University), Ministry of Education and School of Materials Science and Engineering, Jilin University, Changchun 130022, China.

*Corresponding author:

Name: Dr. Lijun Zhao and Dr. Jianshe Lian

E-mail: lijunzhao@jlu.edu.cn; lianjs@jlu.edu.cn

1. Characterizations

The XRD measurement was carried out on a Rigaku-D/max 2500pc X-ray diffractometer equipped with a source of Cu Kα radiation (λ=1.54178 Å) at a step width of 0.02°. X-Ray photoelectron spectroscopy (XPS) with an ESCALAB Mk II spectrometer was used to collect the electronic states of elements in the samples. Cycles of XPS measurements were operated in a high vacuum chamber with a base pressure of 1.33×10^{-6} Pa. The binding energies were corrected by assigning a C 1s peak value to 284.6 eV. Morphologies of the as-synthesized products were characterized with a JSM-6700F field emission scanning electron microscopy (FE-SEM) operated at an acceleration voltage of 10.0 kV. High-resolution transmission electron microscopy (HRTEM) observation was obtained on a JEOL 2100F with an emission voltage of 200 kV. The Brunauer–Emmett–Teller (BET) specific surface areas and Barret–Joyner–Halenda (BJH) pore volumes of the samples were determined by N_2 adsorption-desorption isotherms on a Micromeritics ASAP 2020 M apparatus with all samples degassed at 100°C for 12 h in vacuum before the measurement. An Agilent Cary 50 UV-Vis spectrophotometer was used for determination of CR concentration in the solutions. The hysteresis loops were measured on a VSM-7300 vibrating sample magnetometer (VSM) (Lakeshore, USA) at room temperature. IR spectra of the samples were characterized using a FTIR spectrophotometer (NEXUS, 670) in KBr pellets. The Zeta (ζ)-potential was measured using PALS (phase analysis light scattering) with a zetasizer (Malvern Zetasizer Nano ZS 90, Malvern Instruments). Total concentration of the nanoparticles is 100 mg L^{-1} with aqueous solution. The pH value was adjusted using aqueous solutions of NaOH and HCl. The pH of the Congo red solution was measured with a portable pH meter (SIN-PH173, Hangzhou SinoMeasure Automation technology Co.).

2. Adsorption experiments

The stock solution of CR (1 g L^{-1}) was prepared in deionized water and desired concentrations of the dye were obtained by diluting the same with deionized water. The calibration curve of CR was prepared by measuring the absorbance of different predetermined concentrations of the samples at λ_{max}=497 nm using a UV-Vis spectrophotometer (CR has a maximum absorbency at a wavelength of 497 nm on a UV-Vis spectrophotometer). The amount of adsorbed CR (mg g^{-1}) was calculated based on a mass balance equation as given below:

$$q_e = \frac{(C_0 - C_e) \times V}{W} \quad \text{(S1)}$$

Where q_e is the equilibrium adsorption capacity per gram dry weight of the adsorbent, mg g^{-1}; C_0 is the initial concentration of CR in the solution, mg L^{-1}; C_e is the final or equilibrium concentration of CR in the solution, mg L^{-1}; V is the volume of the solution, L; and W is the dry weight of the nanosized powders, g.

Batch adsorption experiments were carried out by adding 5 mg as-synthesized Co_xNi_{1-x} nanoparticles to 50 mL CR solution under mechanical stirring with a speed of 200 rpm at room temperature.

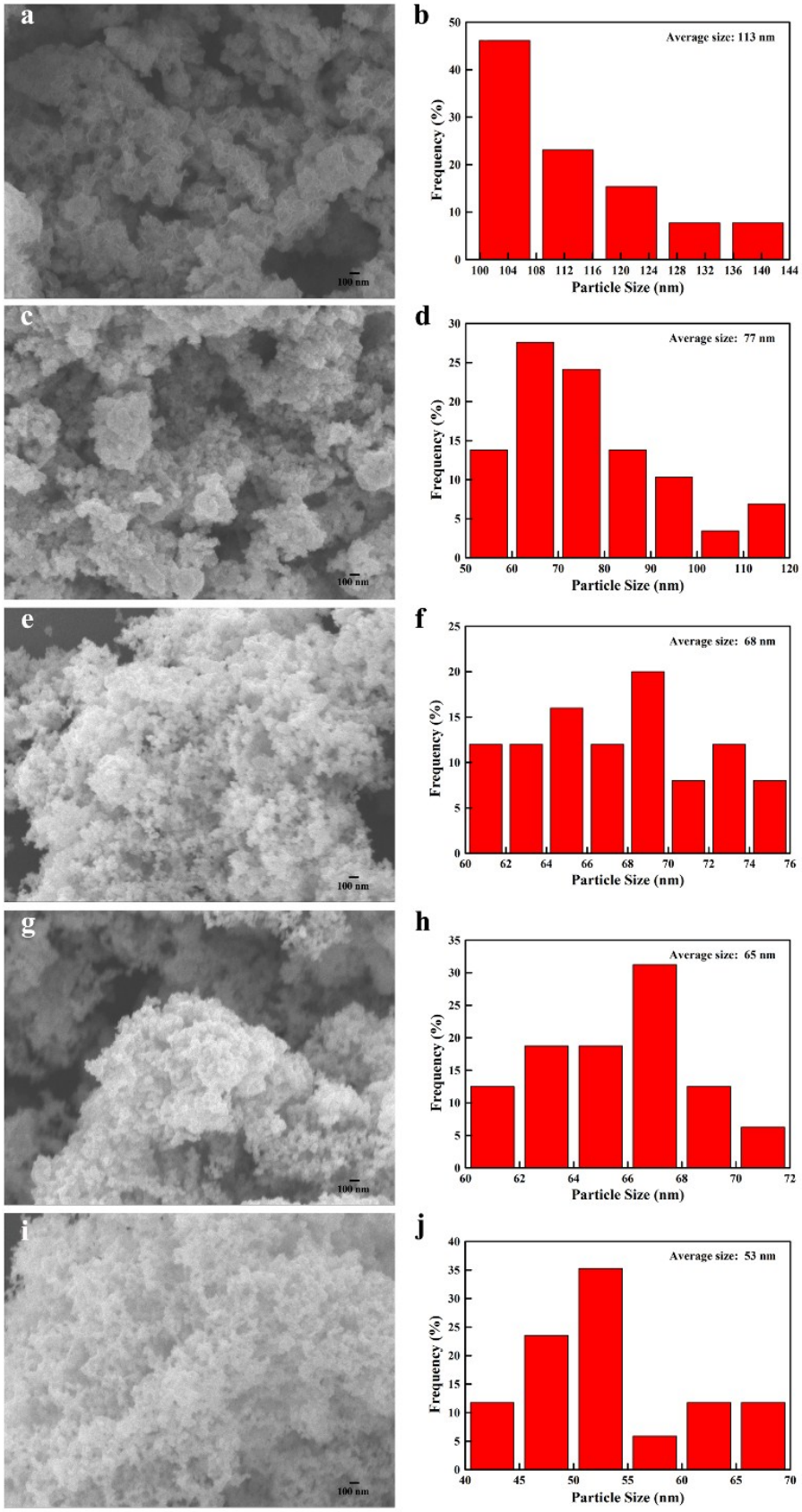

Fig. S1 SEM images and particles sizes distribution of Co_xNi_{1-x} nanoparticles obtained by using different molar ratio: a) and b) Co, c) and d)$Co_{0.8}Ni_{0.2}$, e) and f) $Co_{0.4}Ni_{0.6}$, g) and h) $Co_{0.2}Ni_{0.8}$, i) and j) Ni. (The particle sizes are calculated by Nano Measurer 1.2).

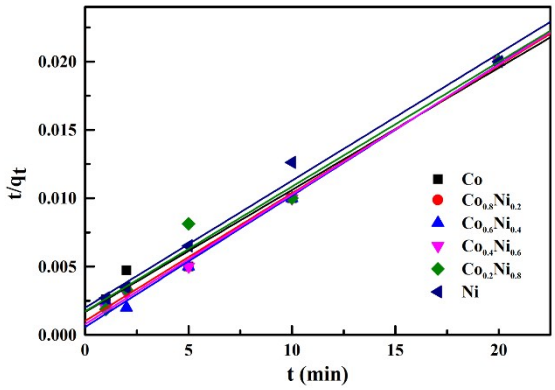

Fig. S2 Pseudo-second-order adsorption kinetic for adsorption of CR on the as-prepared samples. (Initial dye concentration 100 mg L^{-1}, pH is about 7.5, temperature 25 °C)

Table S1 Magnetic Parameters of the synthesized Co_xNi_{1-x} alloy nanoparticles.

Samples	M_s (emu·g^{-1})	M_r (emu·g^{-1})	H_c (Oe)
Co	78.3	20	200
$Co_{0.8}Ni_{0.2}$	46.1	11.5	168
$Co_{0.6}Ni_{0.4}$	42.9	10.3	155
$Co_{0.4}Ni_{0.6}$	32.1	7.8	149
$Co_{0.2}Ni_{0.8}$	18.4	4.8	142
Ni	3.9	1.2	137

Table S2 Adsorption parameters got from kinetic for the adsorption of 100 mg L^{-1} CR on the as-prepared samples.

Samples	$q_{e,exp}$	Pseudo-second-order				
	(mg g^{-1})	K_2(g $mg^{-1}min^{-1}$)	q_e(mg g^{-1})	h(mg g^{-1} min^{-1})	r_2^2	SD
Co	1000	4.8E-04	1119.10	601.14	0.9824	6.9E-05
$Co_{0.8}Ni_{0.2}$	1000	8.6E-04	1070.34	985.24	0.9952	3.7E-05
$Co_{0.6}Ni_{0.4}$	1000	1.6E-03	1039.78	1729.83	0.9946	4.1E-05
$Co_{0.4}Ni_{0.6}$	1000	1.2E-03	1053.01	1330.60	0.9973	2.9E-05
$Co_{0.2}Ni_{0.8}$	1000	4.8E-04	1095.92	576.50	0.9767	8.1E-05
Ni	1000	4.3E-04	1075.37	497.26	0.9888	5.7E-05