SUPPORTING INFORMATION

Effects of metal substitution in transition-metal phosphides $(Ni_{1-x}M'_x)_2P$ (M' = Cr, Fe, Co) studied by X-ray photoelectron and absorption spectroscopy

Peter E. R. Blanchard, Andrew P. Grosvenor, Ronald G. Cavell and Arthur Mar[1]

Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2

[1] Corresponding author. Fax: +1-780-492-8231.
E-mail address: arthur.mar@ualberta.ca (A. Mar).

Table S1. Cell parameters for $(Ni_{1-x}M'_x)_2P$ (M' = Cr, Fe, Co) samples

Sample	Structure type [a]	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)
Cr_2P	Cr_2P-type	6.648(2)	10.458(2)	6.371(1)	443.0(1)
Fe_2P	Fe_2P-type	5.894(1)		3.478(3)	104.64(8)
Co_2P	Co_2P-type	5.674(1)	3.5290(9)	6.6387(8)	132.93(3)
Ni_2P	Fe_2P-type	5.893(4)		3.402(6)	102.3(2)
$(Ni_{0.8}Cr_{0.2})_2P$	Fe_2P-type	5.886(3)		3.396(5)	101.9(2)
$(Ni_{0.5}Cr_{0.5})_2P$	Co_2P-type	5.854(2)	3.555(1)	6.874(3)	142.8(1)
$(Ni_{0.3}Cr_{0.7})_2P$	Co_2P-type	5.878(2)	3.570(1)	6.912(2)	145.07(5)
$(Ni_{0.8}Fe_{0.2})_2P$	Fe_2P-type	5.896(1)		3.367(3)	101.36(7)
$(Ni_{0.5}Fe_{0.5})_2P$	Fe_2P-type	5.878(2)		3.451(3)	103.26(7)
$(Ni_{0.2}Fe_{0.8})_2P$	Fe_2P-type	5.881(2)		3.479(5)	104.2(1)
$(Ni_{0.8}Co_{0.2})_2P$	Fe_2P-type	5.886(2)		3.401(3)	102.0(3)
$(Ni_{0.5}Co_{0.5})_2P$	Fe_2P-type	5.851(6)		3.394(4)	100.6(4)
$(Ni_{0.2}Co_{0.8})_2P$	Co_2P-type	5.701(3)	3.5076(2)	6.6363(6)	132.72(6)

[a] Cr_2P-type, space group *Imm*2; Fe_2P-type, space group $P\bar{6}2m$; Co_2P-type, space group *Pnma*.

Table S2. P $2p_{3/2}$ BEs (eV) for separate $(Ni_{1-x}M'_x)_2P$ (M' = Cr, Fe, Co) samples, or same sample measured at different times

Sample	Run 1	Run 2	Run 3
$(Ni_{0.8}Co_{0.2})_2P$	129.45	129.47	
$(Ni_{0.5}Co_{0.5})_2P$	129.44	129.42	129.39 [a]
$(Ni_{0.2}Co_{0.8})_2P$	129.41	129.39	129.42 [a]
$(Ni_{0.8}Fe_{0.2})_2P$	129.43	129.39	129.42 [a]
$(Ni_{0.5}Fe_{0.5})_2P$	129.39	129.49	129.43 [a]
$(Ni_{0.2}Fe_{0.8})_2P$	129.42	129.33	129.32 [a]
$(Ni_{0.8}Cr_{0.2})_2P$	129.44	129.37	
$(Ni_{0.5}Cr_{0.5})_2P$	129.37	129.32	
$(Ni_{0.3}Cr_{0.7})_2P$	129.23	129.26	

[a] Obtained before Ar^+-ion sputter-cleaning.

Table S3. Metal $2p_{3/2}$ BEs (eV) for separate $(Ni_{1-x}M'_x)_2P$ (M' = Cr, Fe, Co) samples, or same sample measured at different times

Sample	Ni $2p_{3/2}$			M' $2p_{3/2}$		
	Run 1	Run 2	Run 3	Run 1	Run 2	Run 3
$(Ni_{0.8}Co_{0.2})_2P$	852.93	853.02		778.10	778.14	
$(Ni_{0.5}Co_{0.5})_2P$	852.91	852.88	852.94 [a]	778.14	778.17	778.11 [a]
$(Ni_{0.2}Co_{0.8})_2P$	852.96	853.03	853.05 [a]	778.23	778.30	778.28 [a]
$(Ni_{0.8}Fe_{0.2})_2P$	852.91	852.86	852.85 [a]	706.62	706.64	706.71 [a]
$(Ni_{0.5}Fe_{0.5})_2P$	853.05	853.01	852.98 [a]	706.86	706.83	706.92 [a]
$(Ni_{0.2}Fe_{0.8})_2P$	853.09	853.04	853.08 [a]	706.74	706.84	706.81 [a]
$(Ni_{0.8}Cr_{0.2})_2P$	852.92	852.96		573.98	574.09	
$(Ni_{0.5}Cr_{0.5})_2P$	853.11	853.16		574.01	574.09	
$(Ni_{0.3}Cr_{0.7})_2P$	853.20	853.12		574.08	573.99	

[a] Obtained before Ar^+-ion sputter-cleaning.

Figure S1

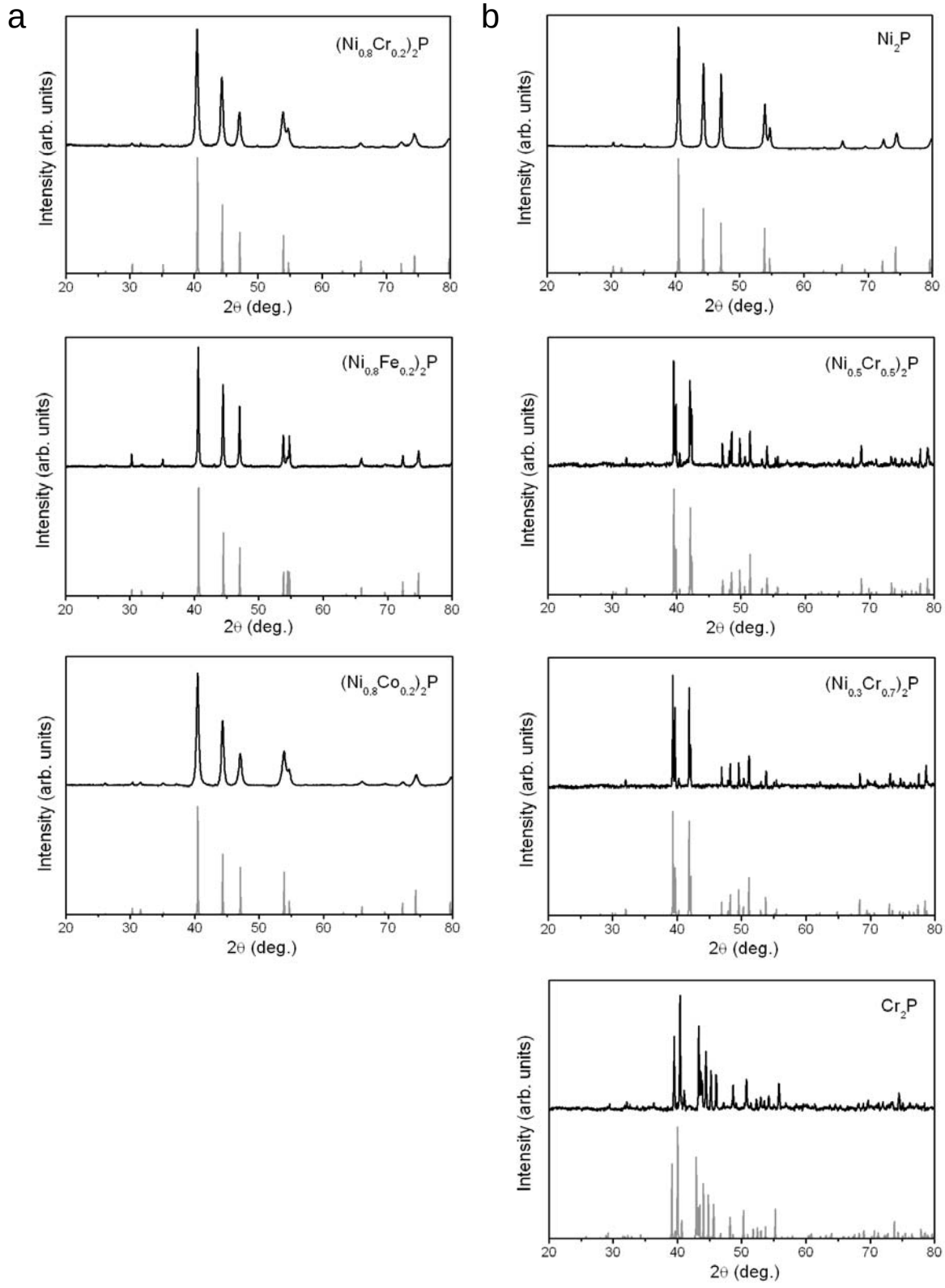


Figure S2

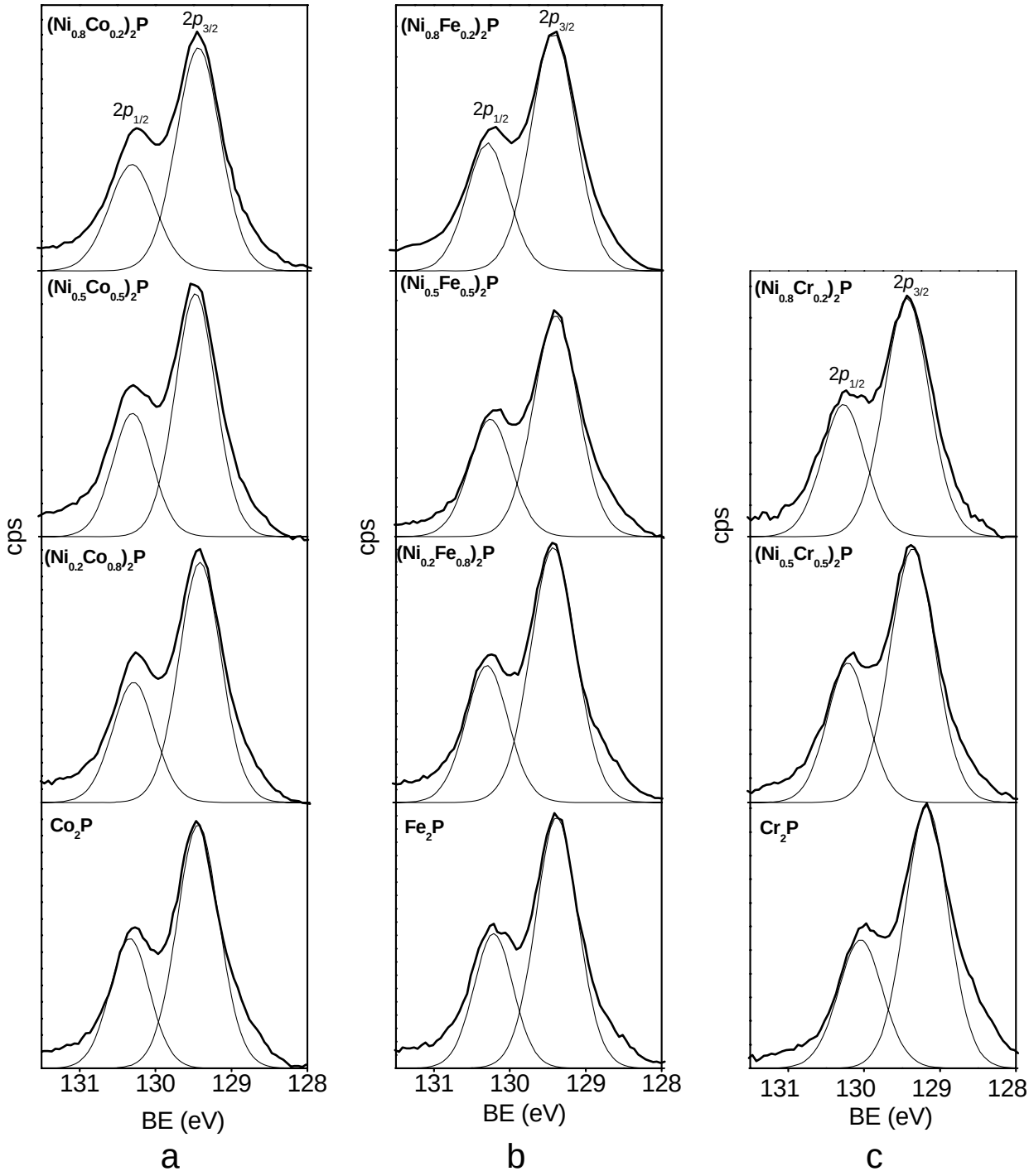

(Ni0.8Co0.2)2P
2p3/2
2p1/2
(Ni0.5Co0.5)2P
(Ni0.2Co0.8)2P
Co2P
(Ni0.8Fe0.2)2P
(Ni0.5Fe0.5)2P
(Ni0.2Fe0.8)2P
Fe2P
(Ni0.8Cr0.2)2P
(Ni0.5Cr0.5)2P
Cr2P
cps
131
130
129
128
BE (eV)
a
b
c

Figure S3

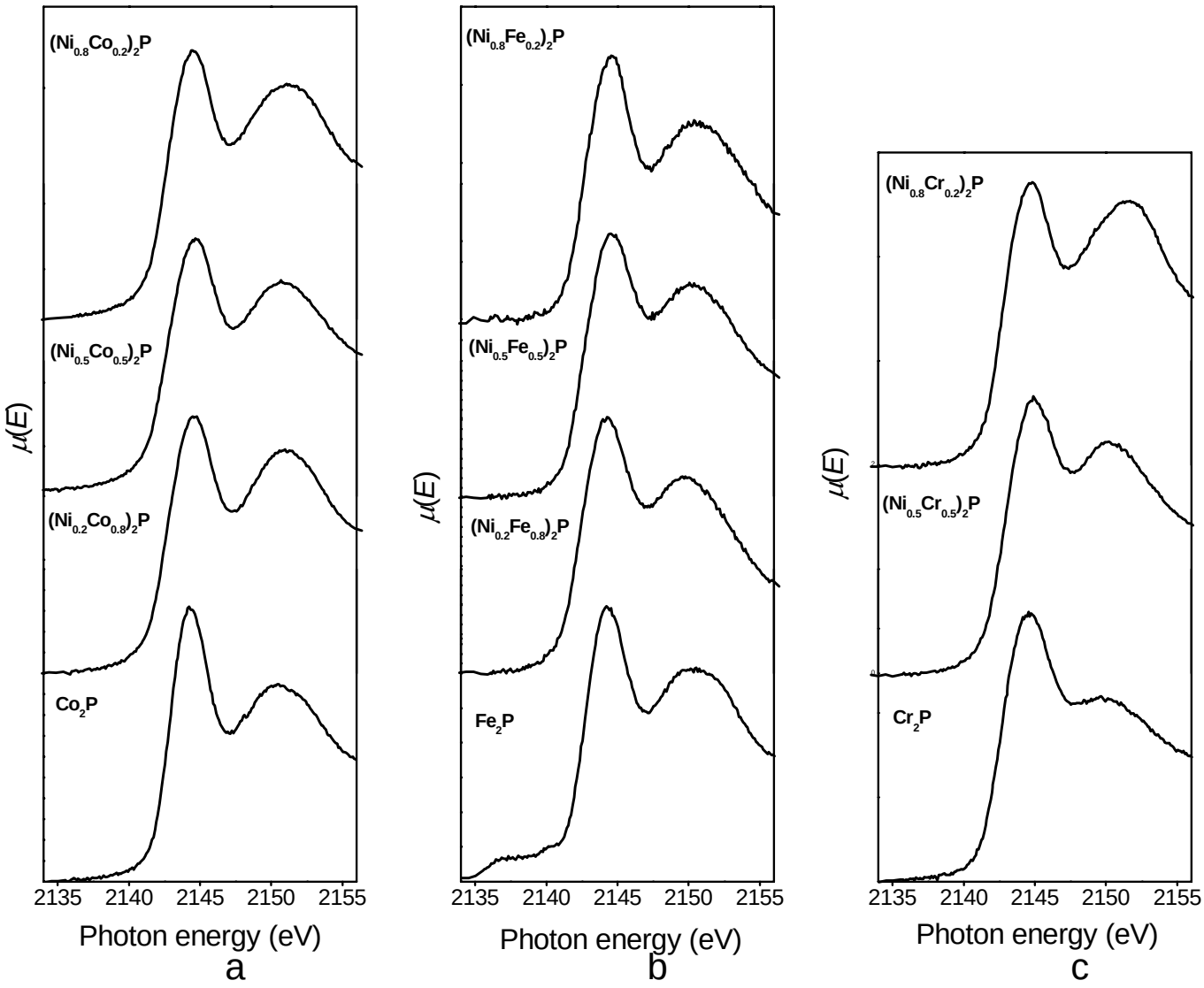


Figure S4a

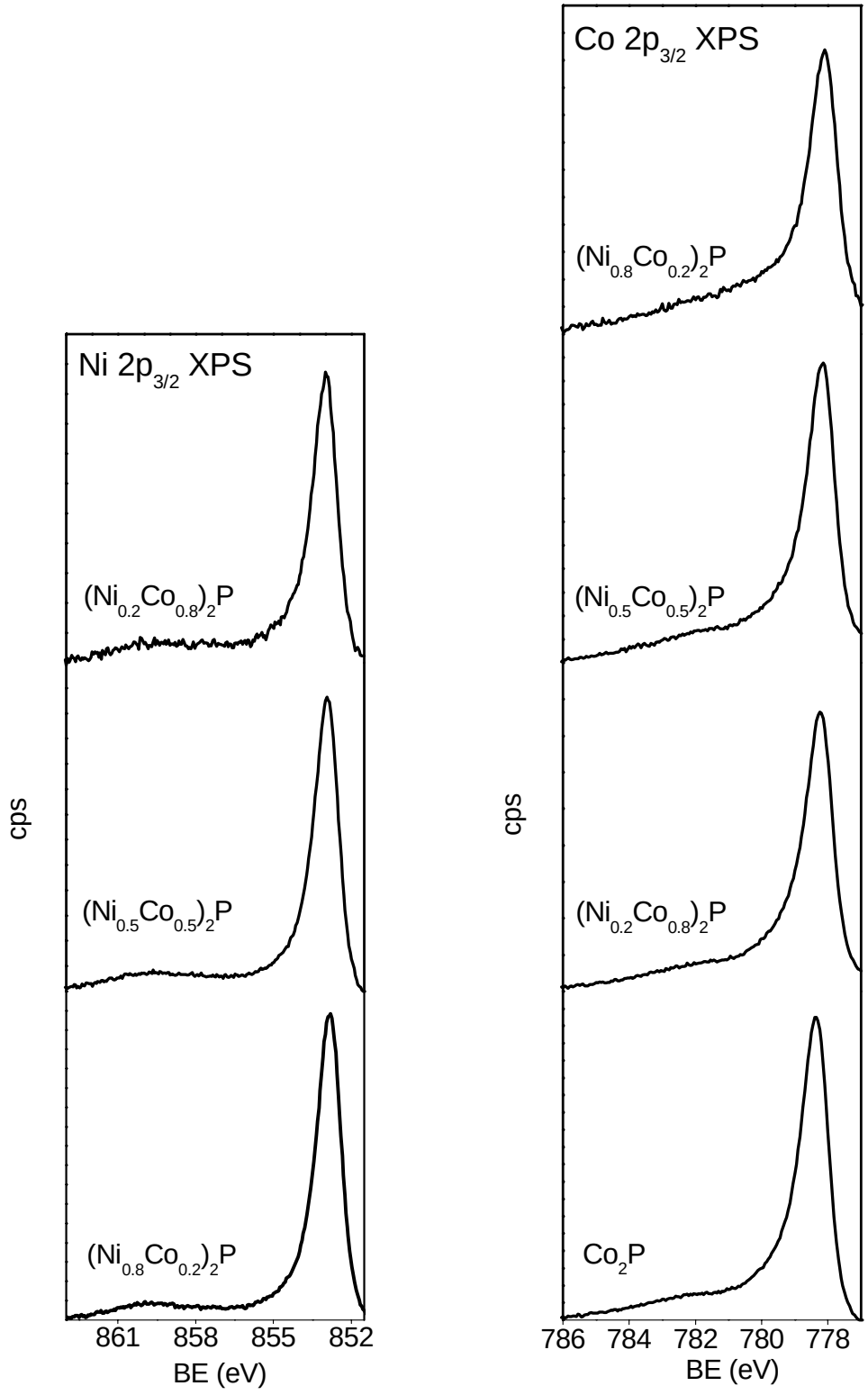


Figure S4b

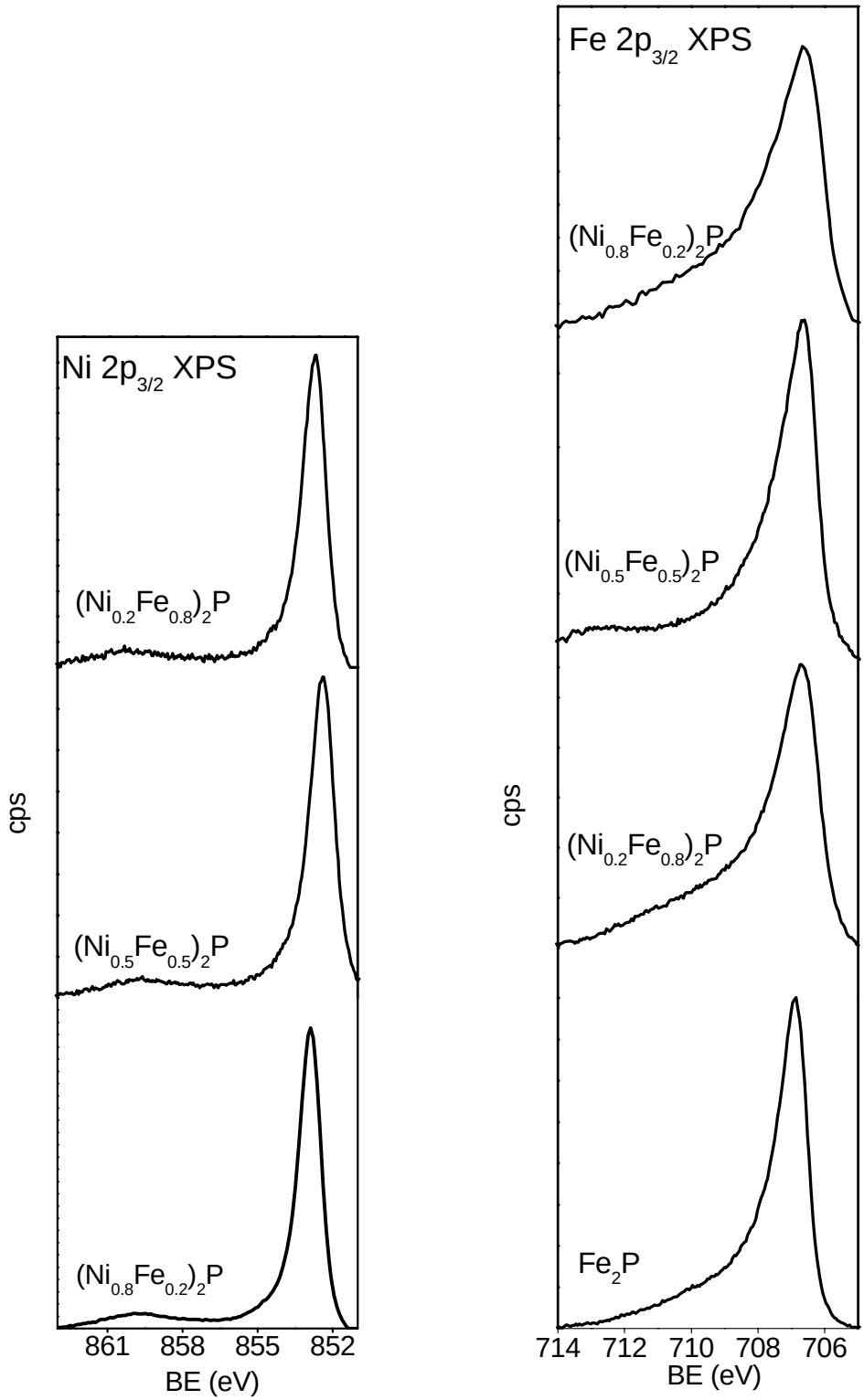


Figure S4c

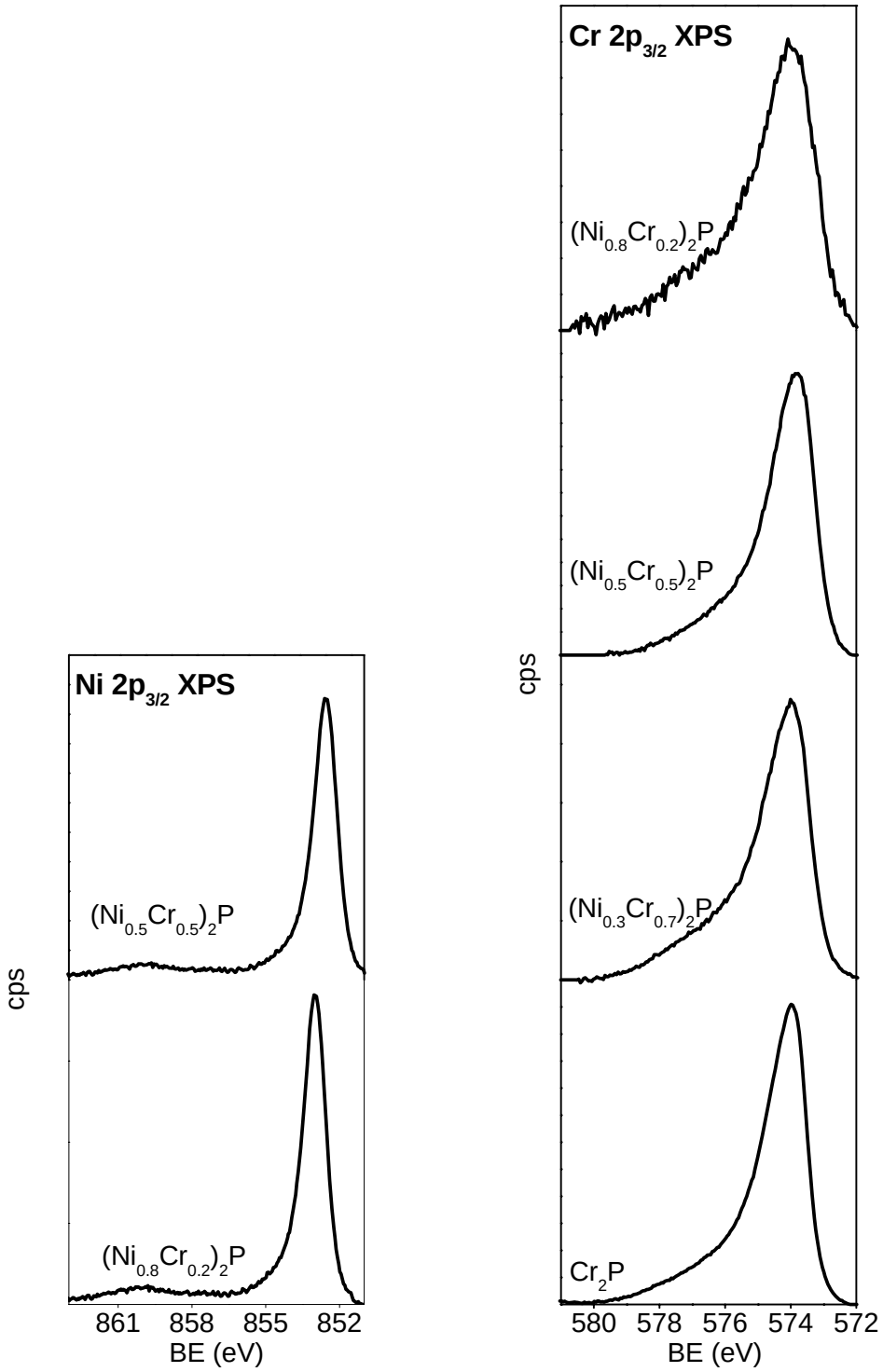
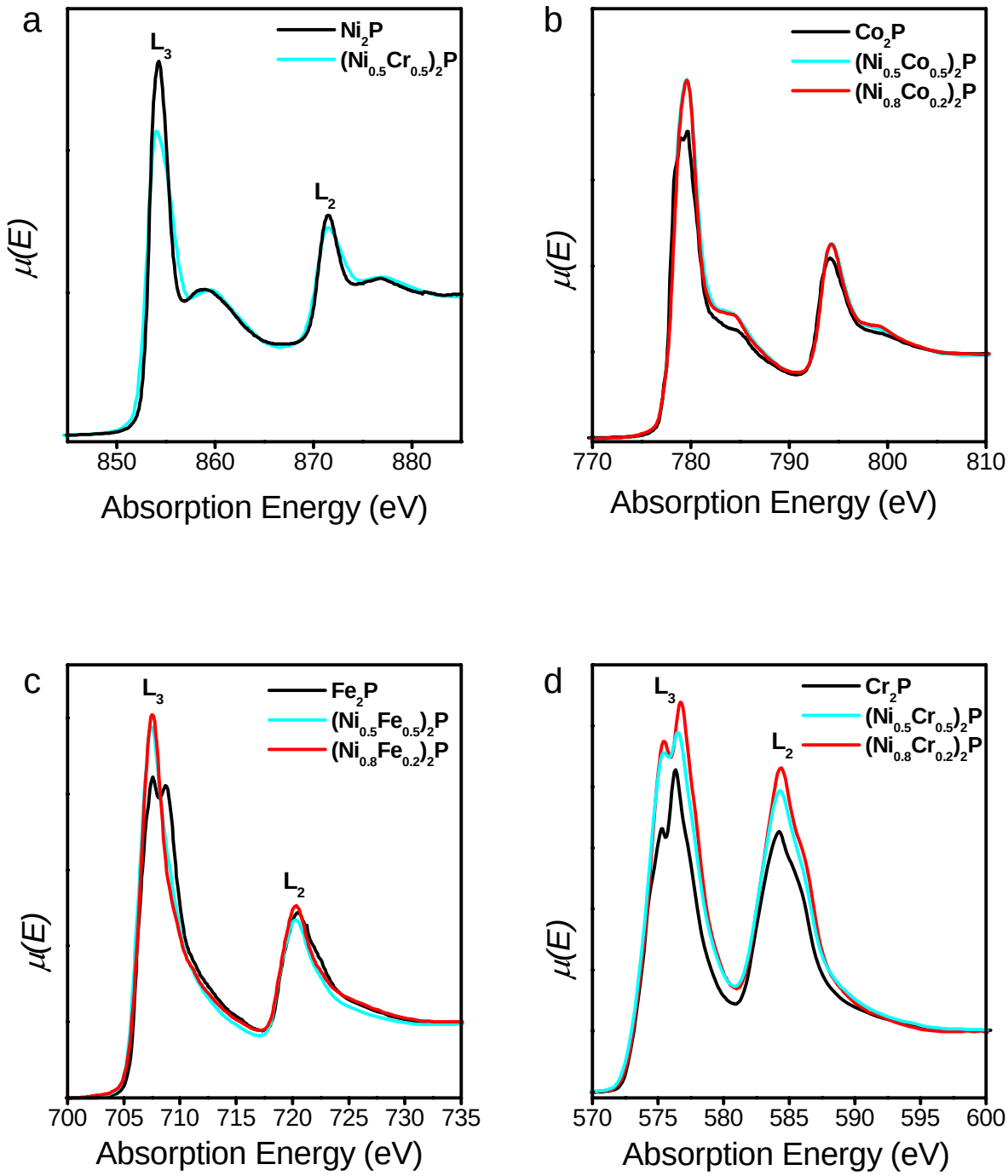

Ni 2p3/2 XPS
(Ni0.5Cr0.5)2P
(Ni0.8Cr0.2)2P
cps
861 858 855 852
BE (eV)
Cr 2p3/2 XPS
(Ni0.8Cr0.2)2P
(Ni0.5Cr0.5)2P
(Ni0.3Cr0.7)2P
Cr2P
cps
580 578 576 574 572
BE (eV)

Figure S5


a
Ni2P
(Ni0.5Cr0.5)2P
L3
L2
μ(E)
850 860 870 880
Absorption Energy (eV)
b
Co2P
(Ni0.5Co0.5)2P
(Ni0.8Co0.2)2P
μ(E)
770 780 790 800 810
Absorption Energy (eV)
c
Fe2P
(Ni0.5Fe0.5)2P
(Ni0.8Fe0.2)2P
L3
L2
μ(E)
700 705 710 715 720 725 730 735
Absorption Energy (eV)
d
Cr2P
(Ni0.5Cr0.5)2P
(Ni0.8Cr0.2)2P
L3
L2
μ(E)
570 575 580 585 590 595 600
Absorption Energy (eV)