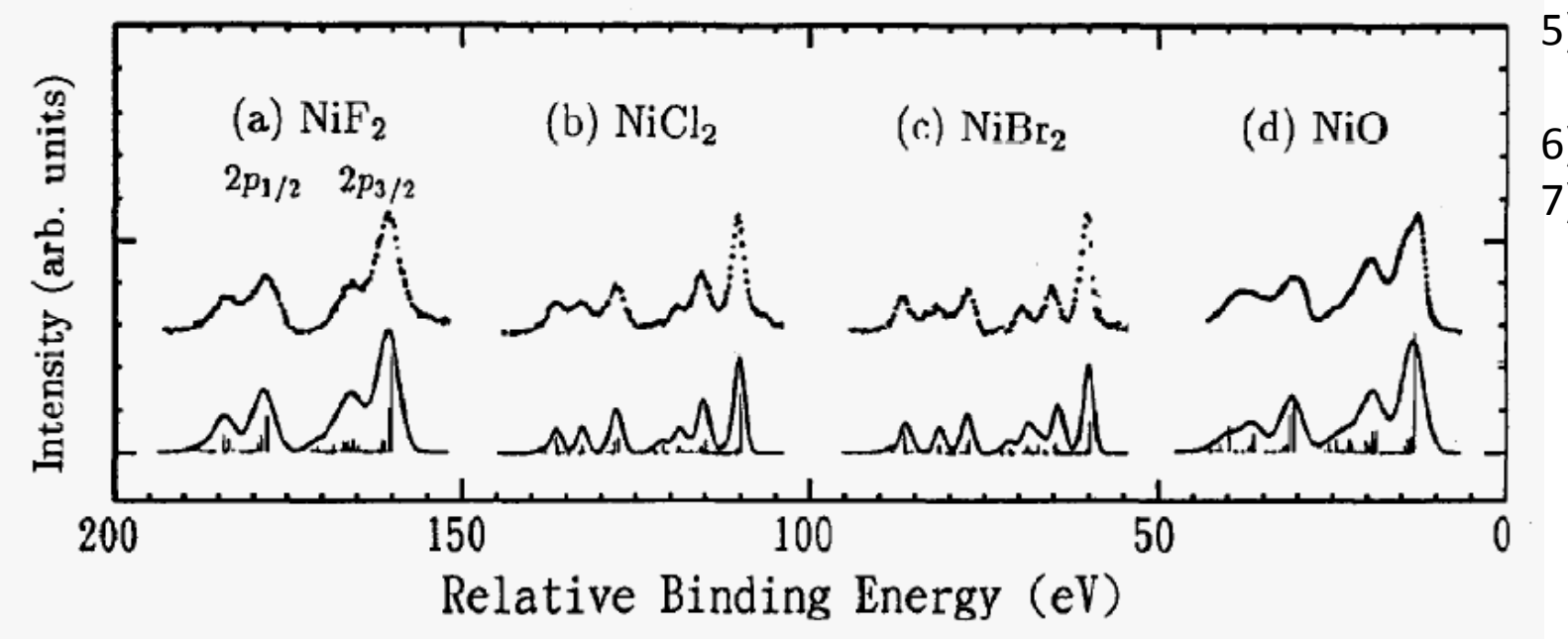
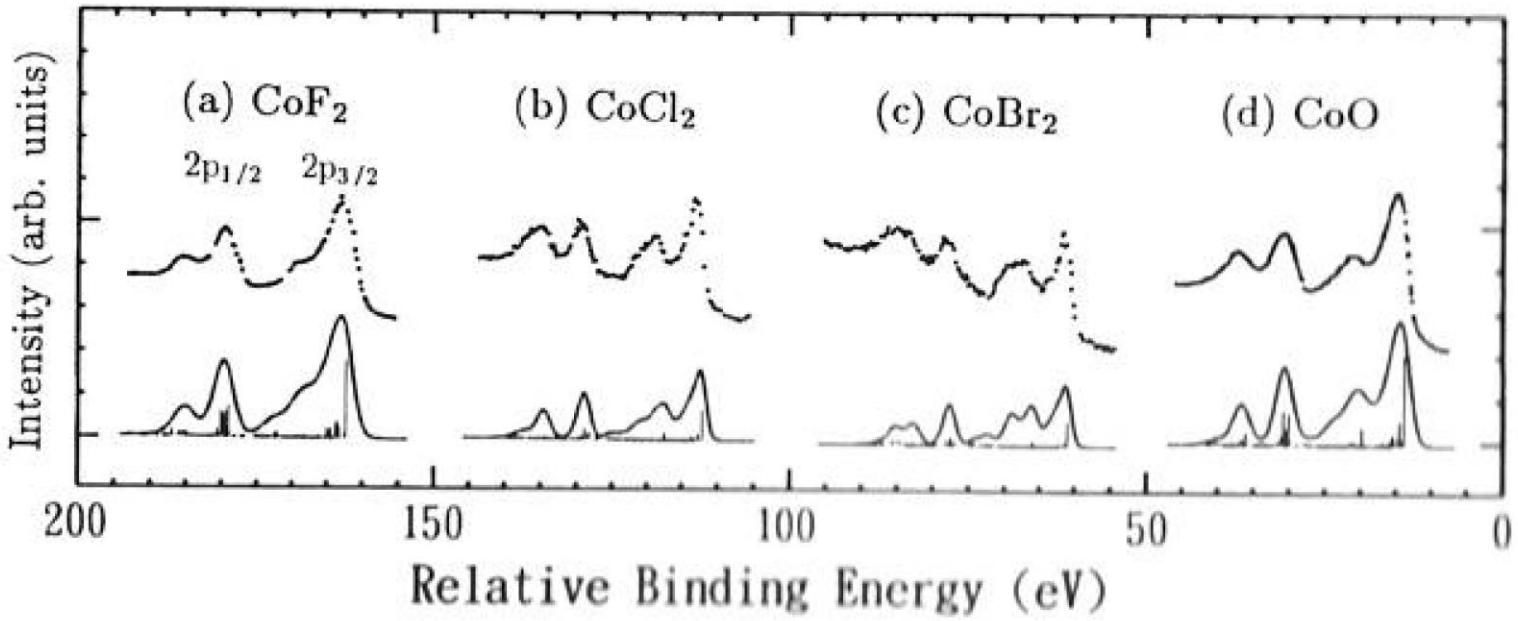
		Δ	Veg	Vt2g	Udd	Upd
Ni2+ 3d8	NiF2	4.3	2.0	1.0	7.3	7.5
	NiCl2	1.3	1.7	0.85	7.3	7.5
	NiBr2	0.3	1.4	0.7	7.3	7.5
	NiO	2.0	2.0	1.0	7.3	7.5
Co2+ 3d7	CoF2	5.0	2.0	1.0	7.0	7.0
	CoCl2	2.0	1.7	0.85	7.0	7.0
	CoBr2	1.0	1.4	0.7	7.0	7.0
	CoO	2.5	2.0	1.0	7.0	7.0



Calculate the Ni2p XPS of Ni2+
Use Gaussian broadening of 3 eV

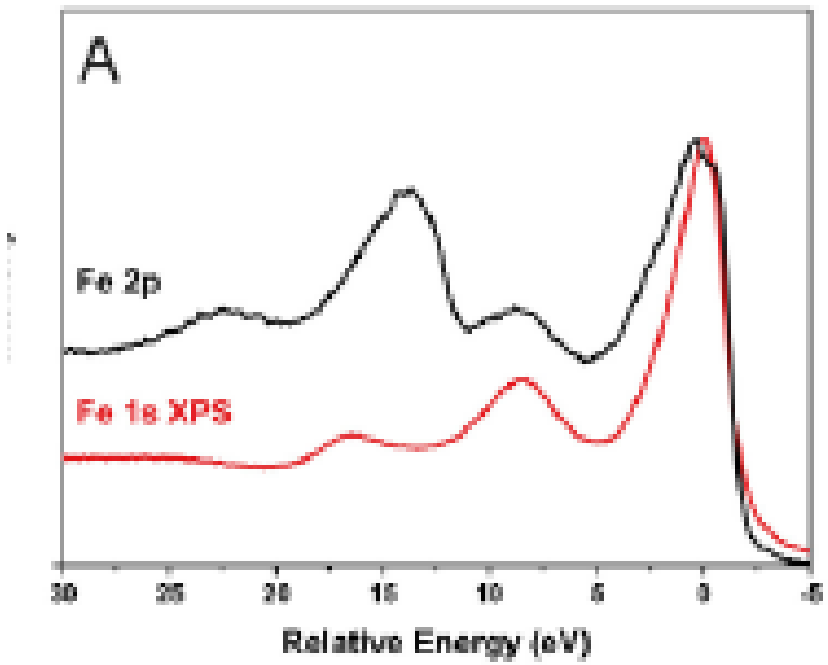
1) Consider only Slater Integrals and spin-orbit coupling
2) Add a cubic crystal field. Use 10Dq=1. Does the simulation improve?
3) Add charge transfer calculations (2 configurations). Does the simulation improve?
4) Add charge transfer calculations (3 configurations)
5) Add charge transfer calculations (4configurations)
6) What is the simulation?
7) Try to find the best delta for each compound.

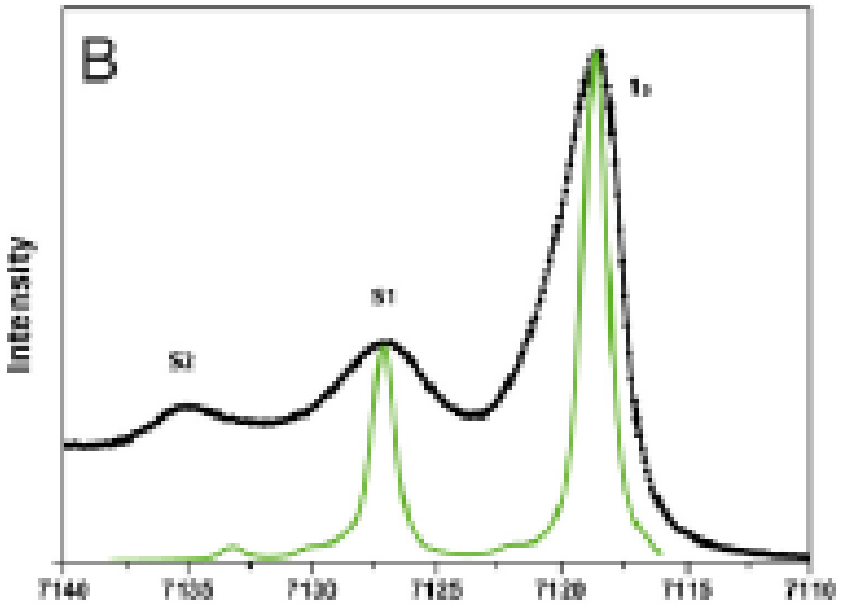
		Δ	Veg	Vt2g	Udd	Upd
Ni2+ 3d8	NiF2	4.3	2.0	1.0	7.3	7.5
	NiCl2	1.3	1.7	0.85	7.3	7.5
	NiBr2	0.3	1.4	0.7	7.3	7.5
	NiO	2.0	2.0	1.0	7.3	7.5
Co2+ 3d7	CoF2	5.0	2.0	1.0	7.0	7.0
	CoCl2	2.0	1.7	0.85	7.0	7.0
	CoBr2	1.0	1.4	0.7	7.0	7.0
	CoO	2.5	2.0	1.0	7.0	7.0



Calculate the Co2p XPS of Co2+
Use Gaussian broadening of 3 eV

1) Try to find the best delta for each compound.





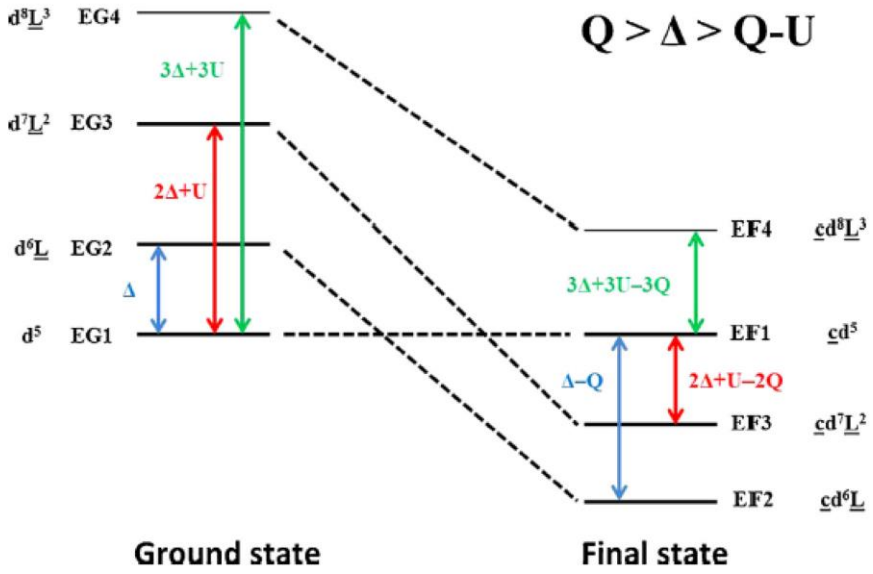
Charge transfer effects in XPS

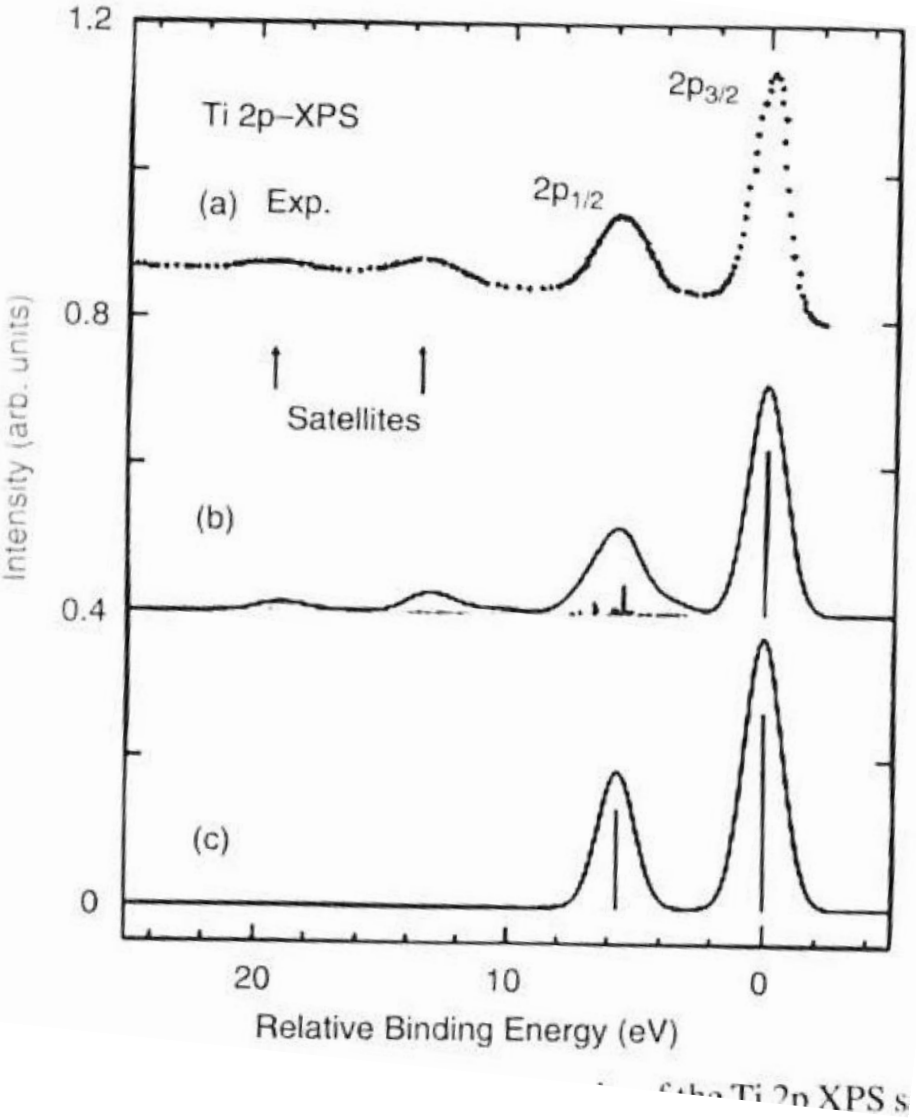
1s and 2p XPS of Fe2O3

Fe3+ 3d5

1) Calculate the 1s XPS of Fe3+ . Try to find Udd and Δ.
2) How the Fe 2p XPS changes when Q = Upd is varied from 0 to 10?

	Δ	Veg	Vt2g	Udd	Upd
	3	2.0	1.0	6	7.5





Charge transfer effects in XPS

2p XPS of TiO2

Ti4+ 3d0

1) Calculate the 2p XPS of Ti4+ . How the Ti 2p XPS changes when Q = Upd is varied from 0 to 10?

	Δ	Veg	Vt2g	Udd	Upd
	3	3.0	1.5	4	6