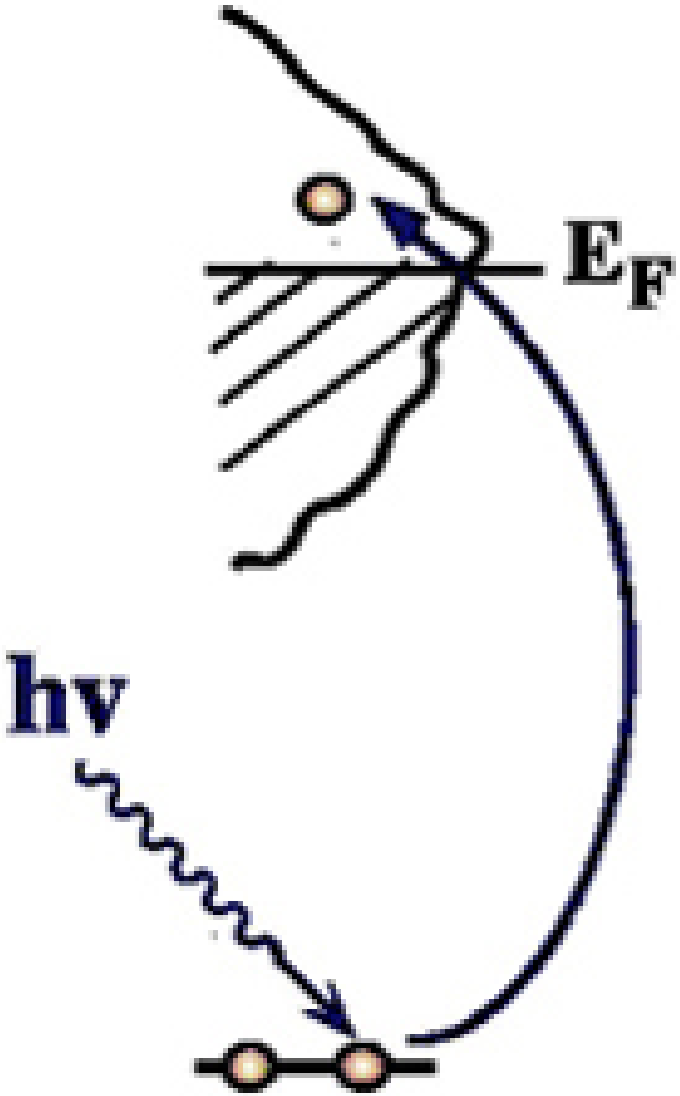
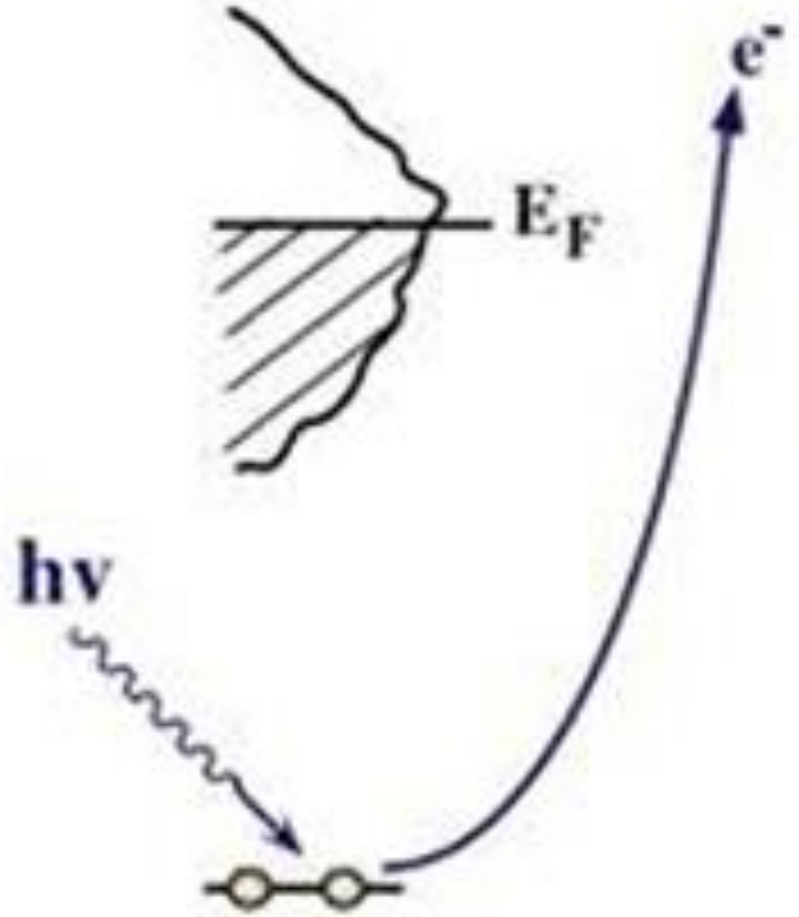
XPS

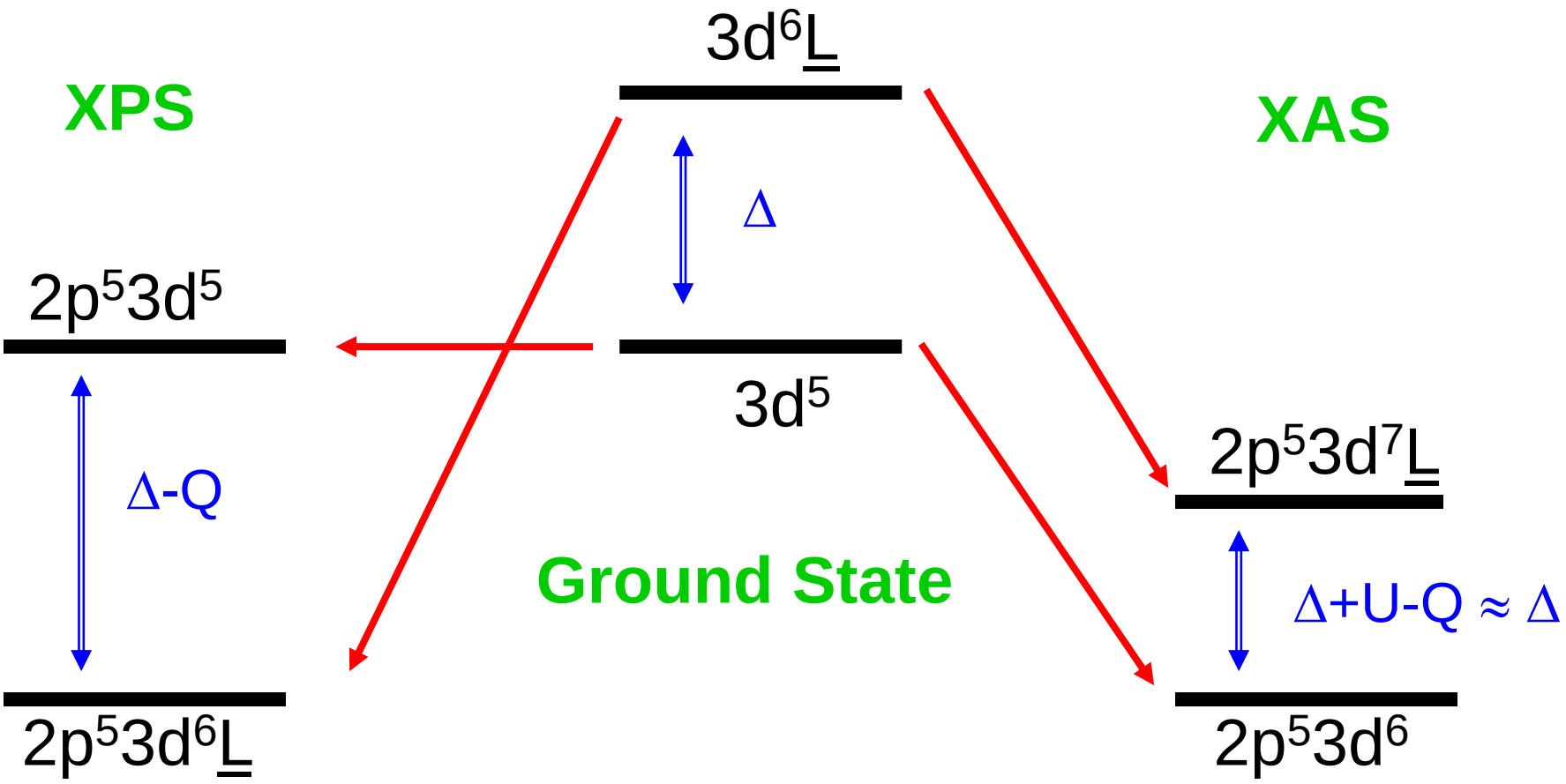
XAS and XPS



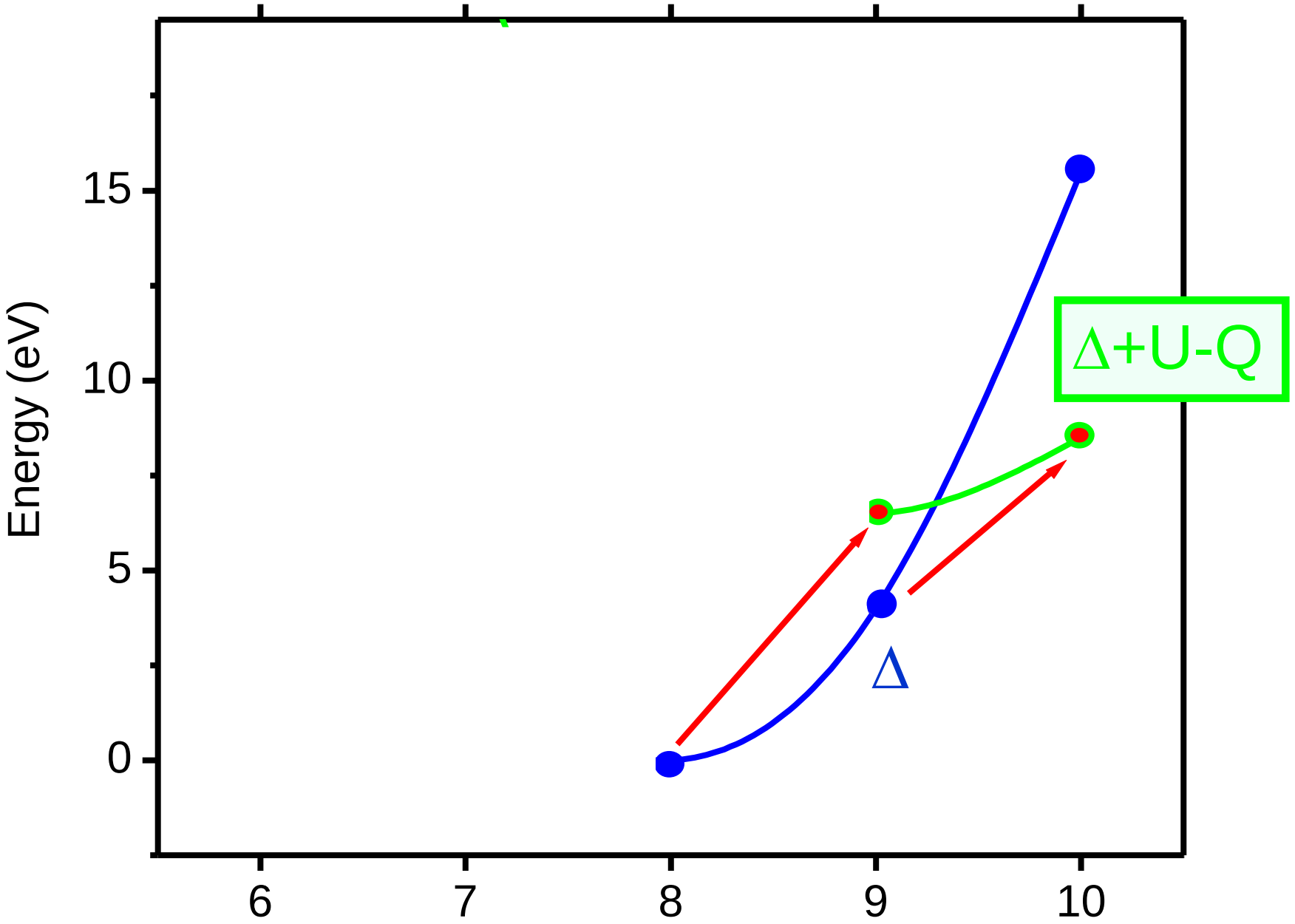


Charge transfer effects in XAS and XPS

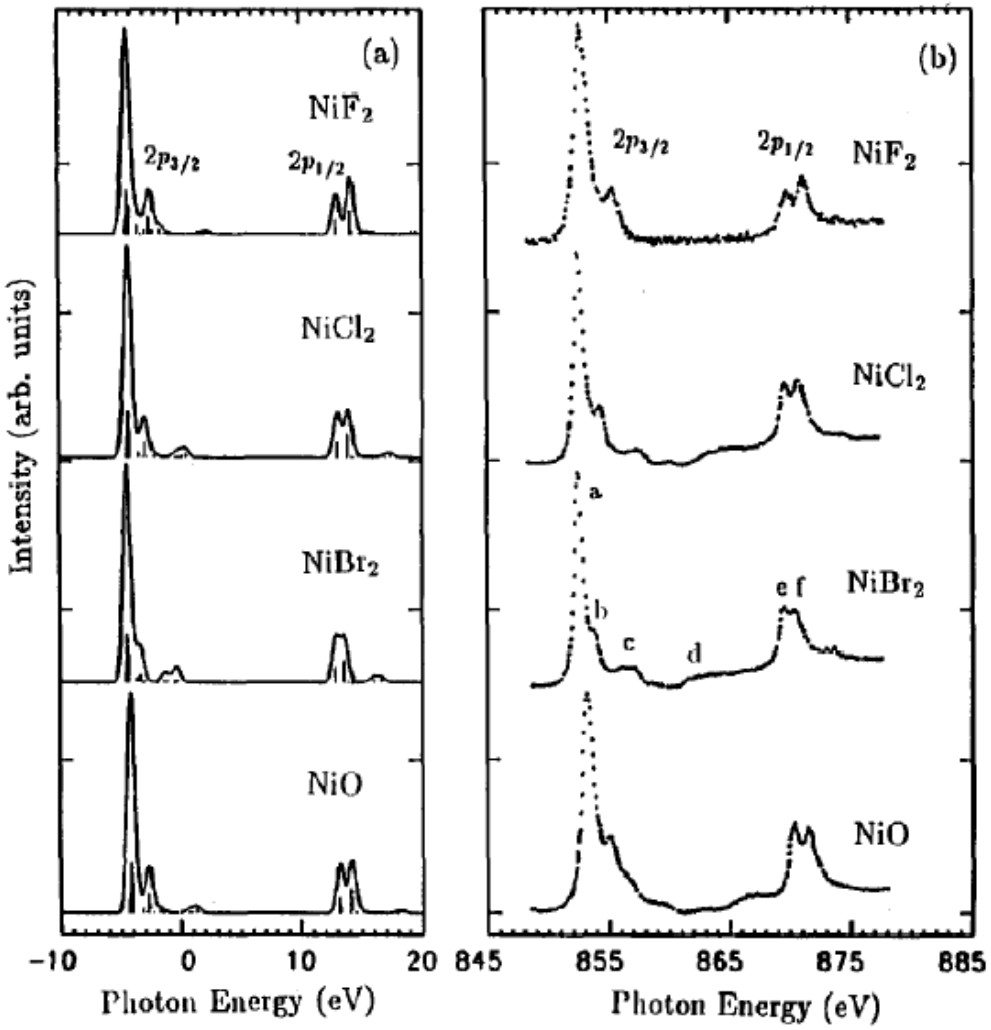
- Transition metal oxide: Ground state: $3d^5 + 3d^6\underline{L}$
- Energy of $3d^6\underline{L}$: Charge transfer energy Δ



Charge transfer effects in XAS



Charge transfer effects in XAS

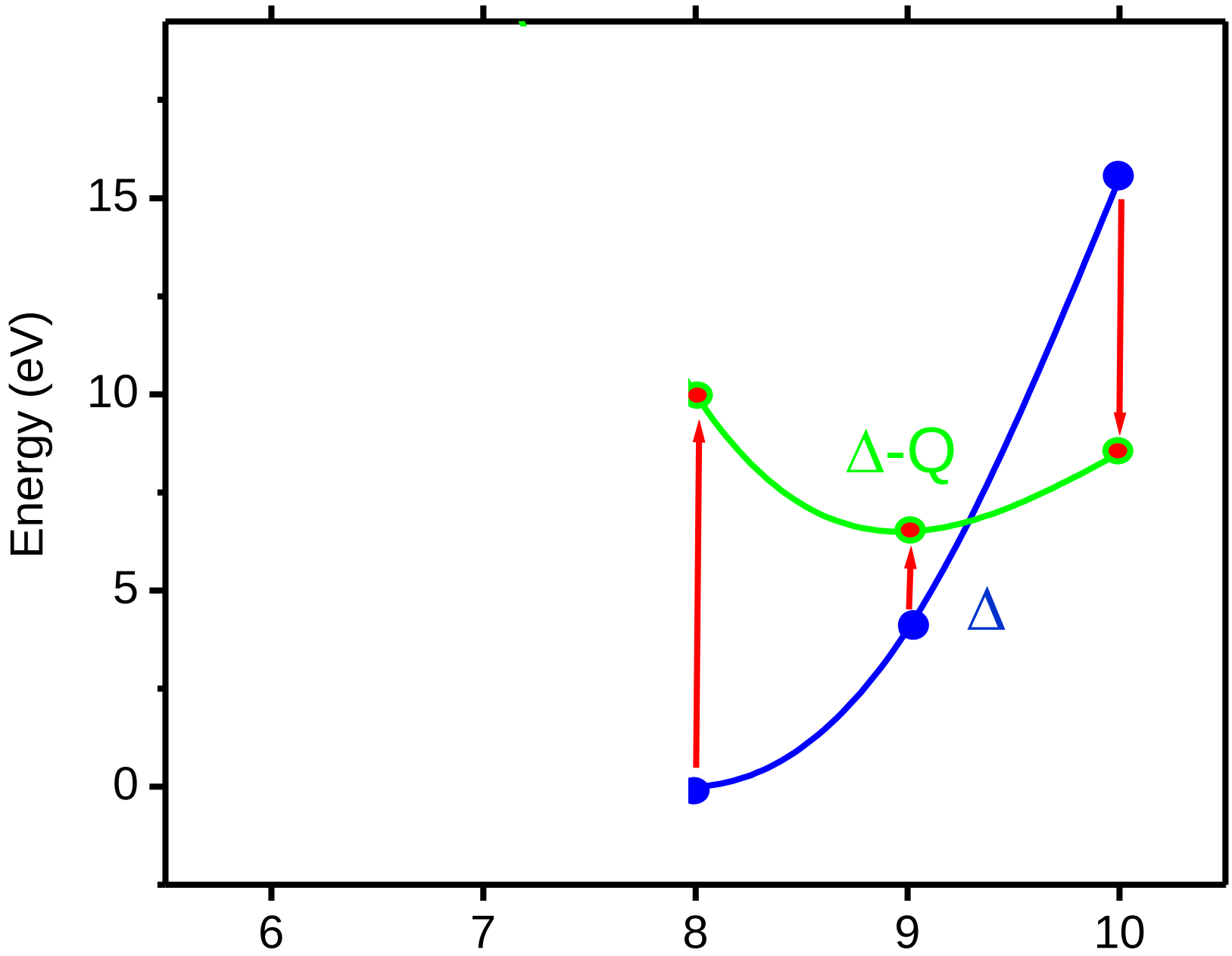


XAS = neutral

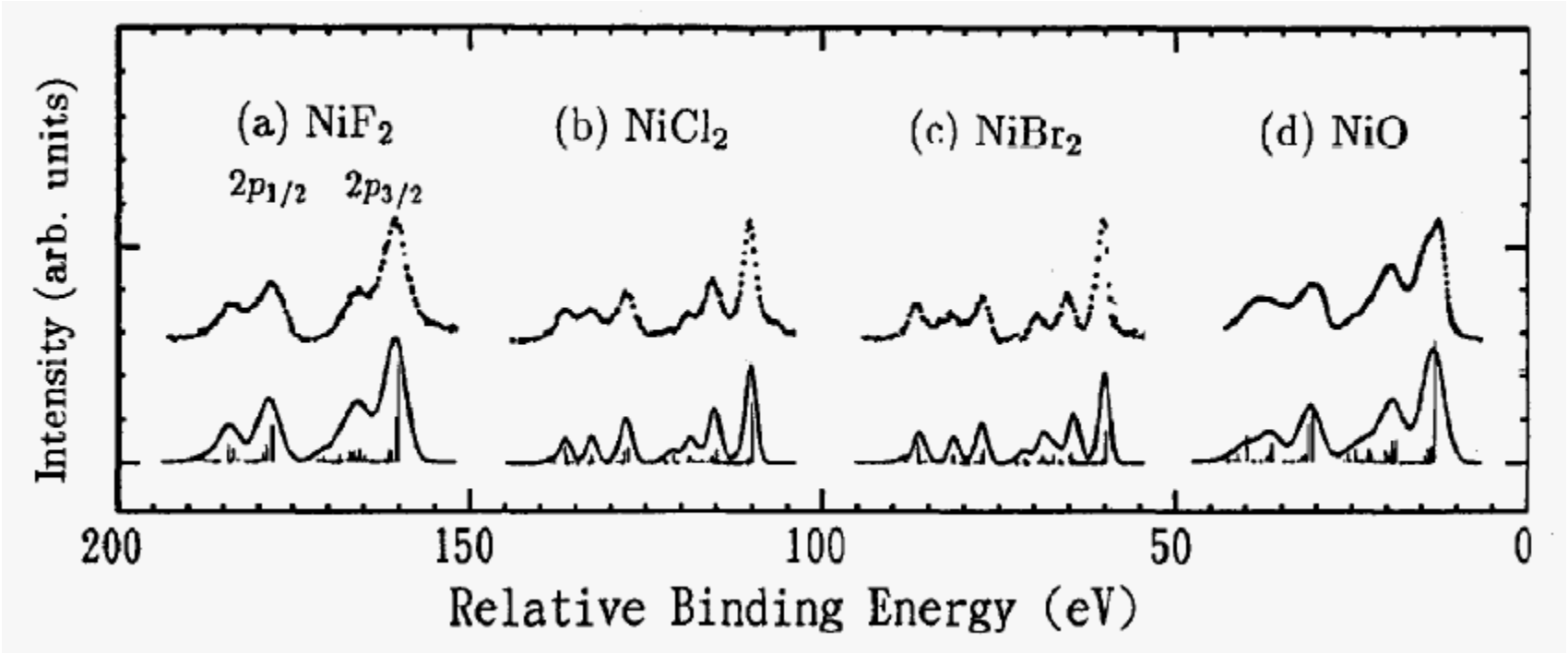
Self screened

Small charge transfer satellites

Charge transfer effects in XPS



Charge transfer effects in XPS



XAS = neutral

Self screened

Small charge transfer satellites

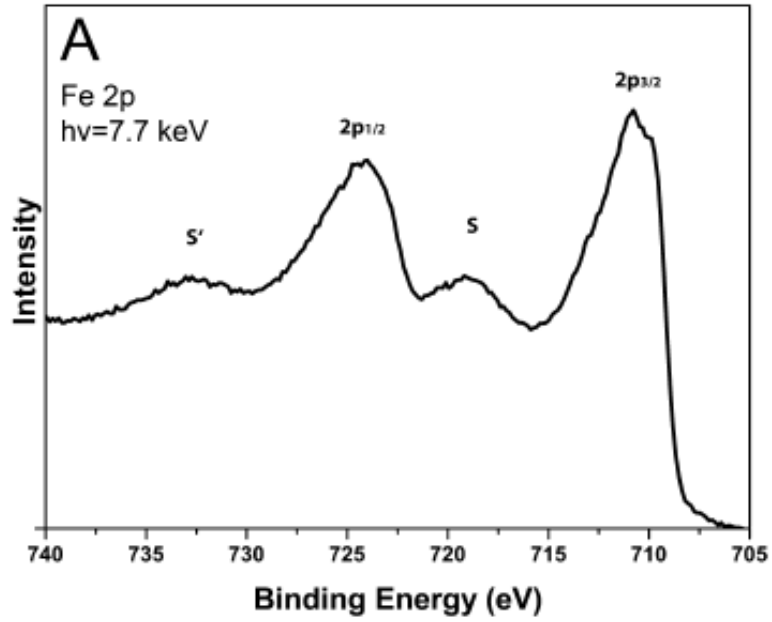
XPS = ionising

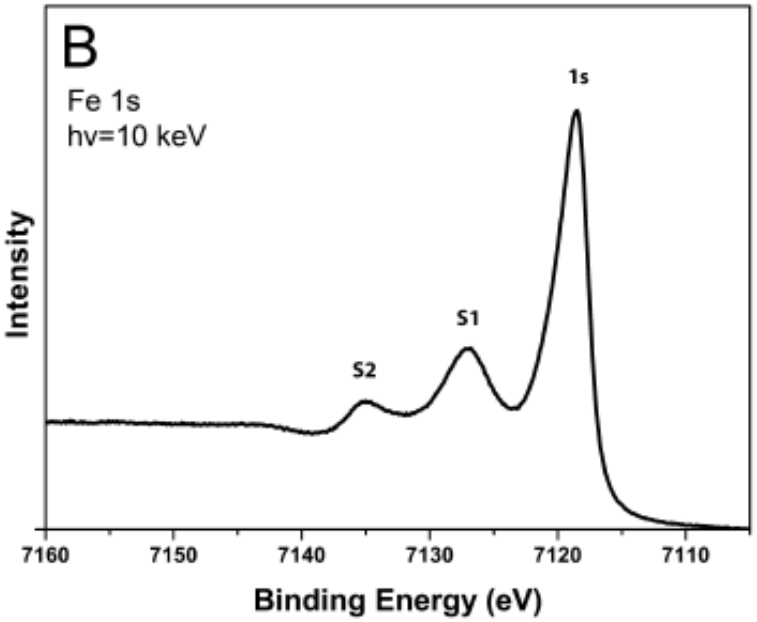
Large screening

Large charge transfer satellites

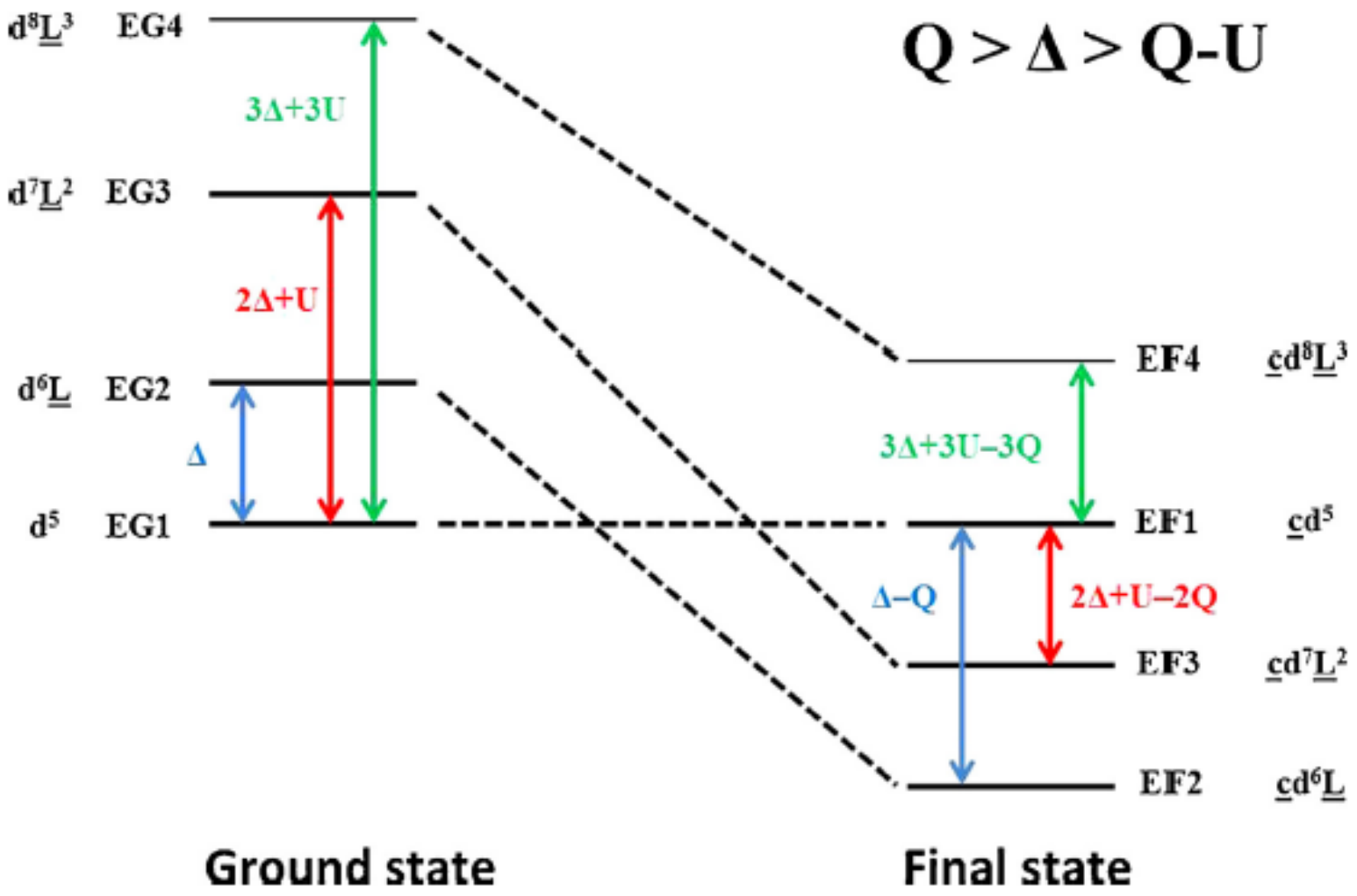
1s and 2p XPS of Fe2O3

1s and 2p XPS of Fe2O3

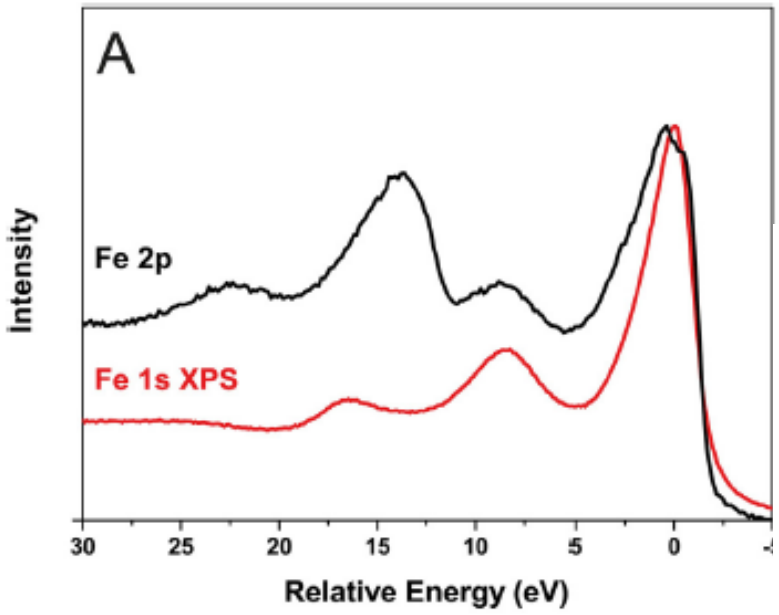


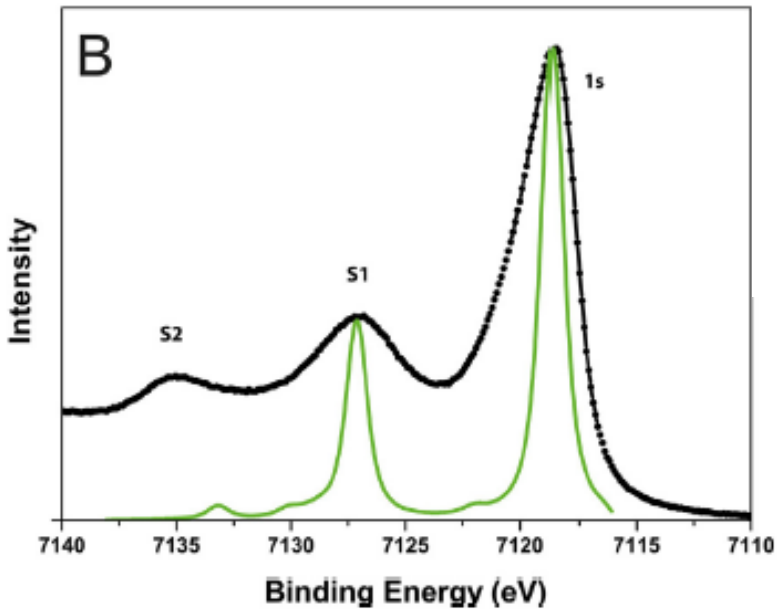


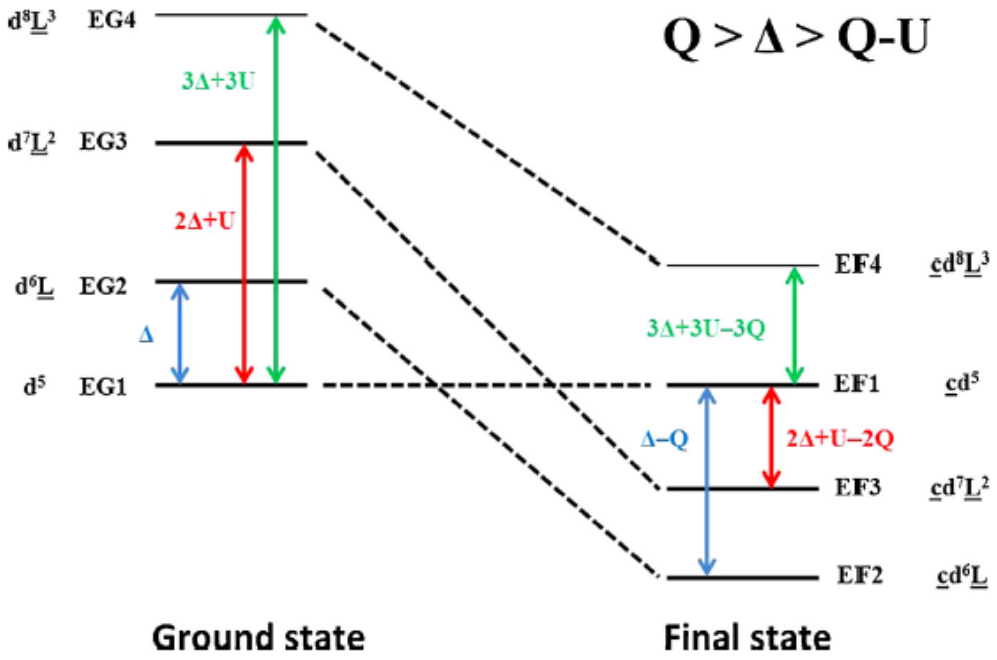
1s and 2p XPS of Fe2O3



1s and 2p XPS of Fe2O3

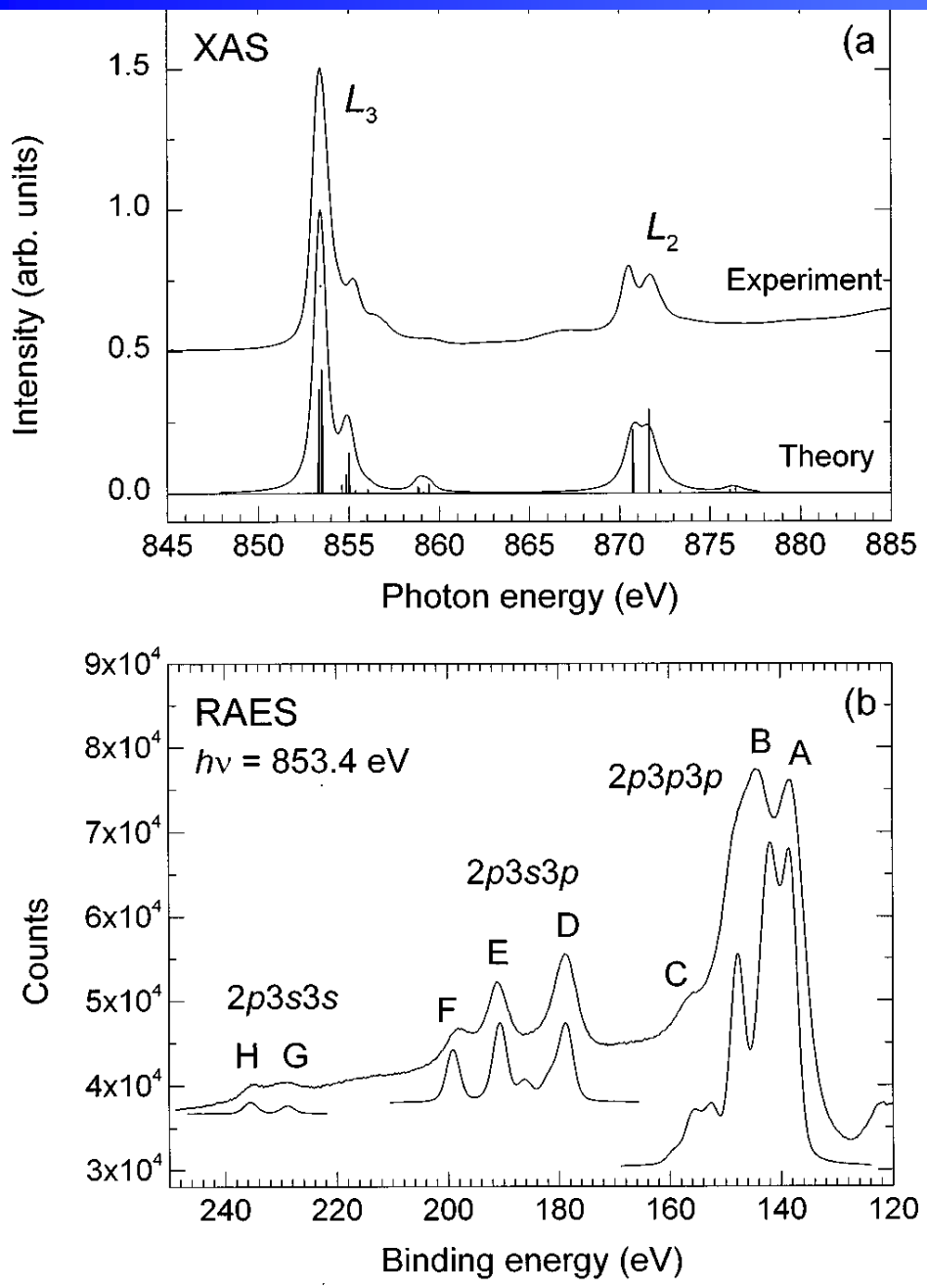






Resonant Auger of NiO

Resonant Auger of NiO



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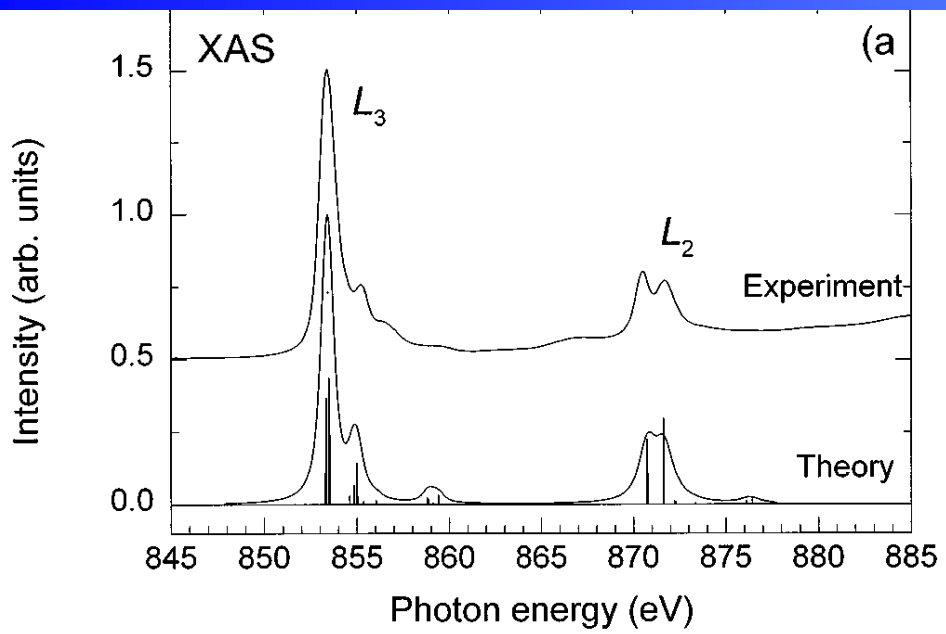
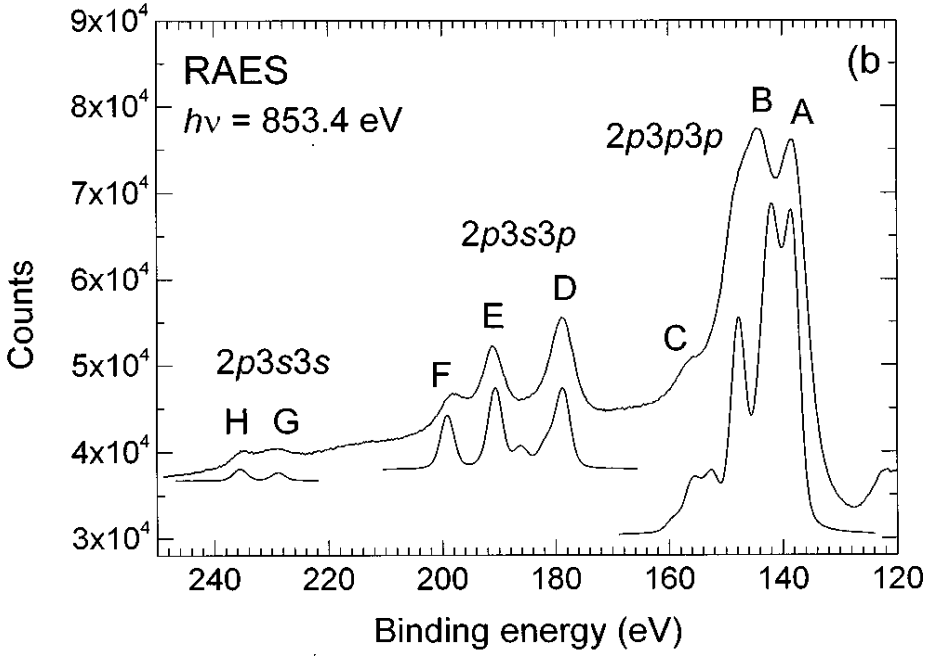
Resonant Auger of NiO



$3d^8 \rightarrow 2p^5 3d^9$



$2p^5 3d^9 \rightarrow 3s^0 3d^9 \varepsilon$

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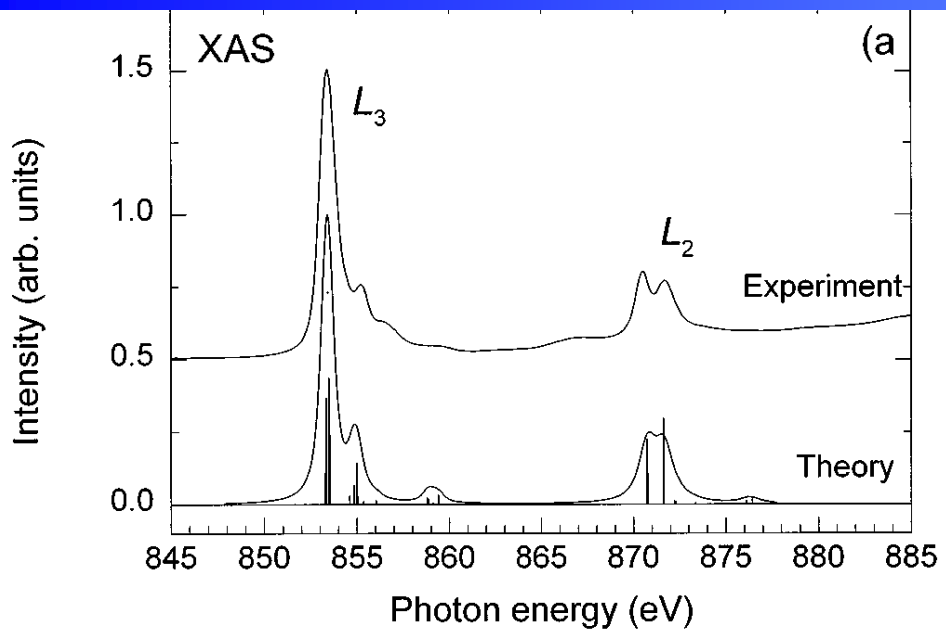
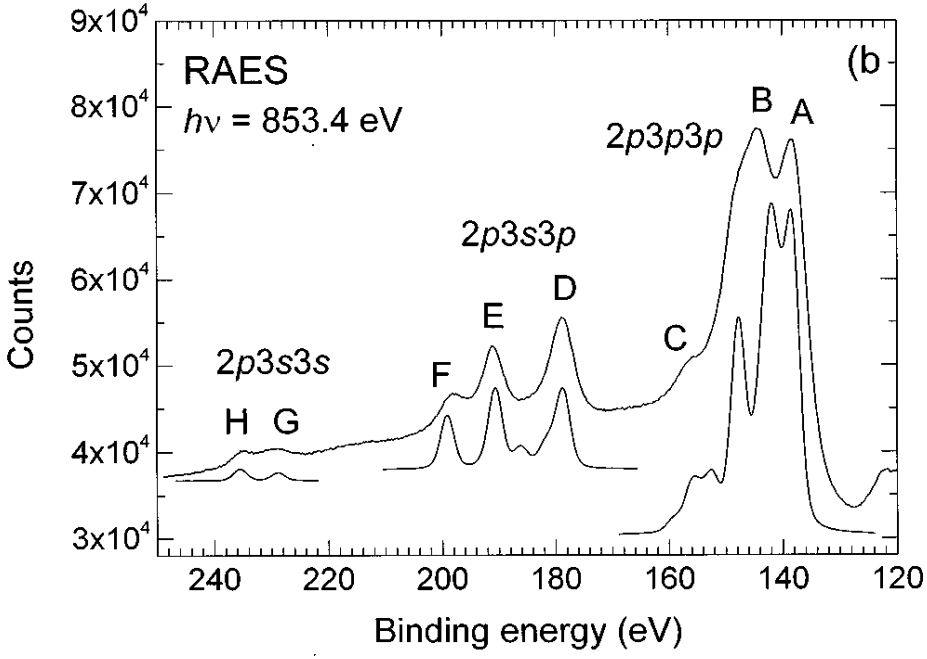
Resonant Auger of NiO



$3d^8 \rightarrow 2p^5 3d^9$

$3d^9\underline{L} \rightarrow 2p^5 3d^{10}\underline{L}$



$2p^5 3d^9 \rightarrow 3s^0 3d^9 \varepsilon$

$2p^5 3d^{10}\underline{L} \rightarrow 3s^0 3d^{10} \varepsilon$

<u>ONLY 2 PEAKS</u>

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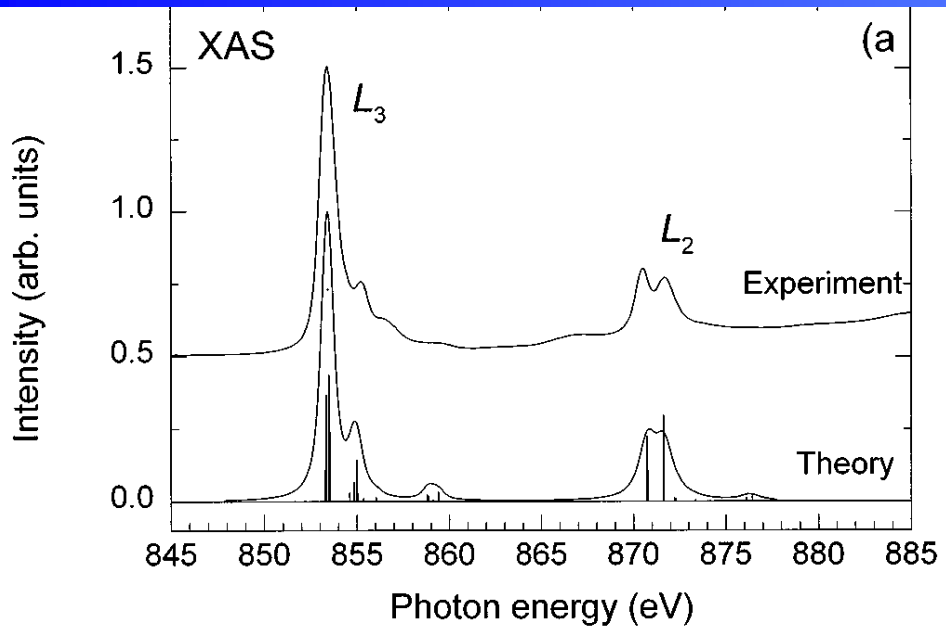
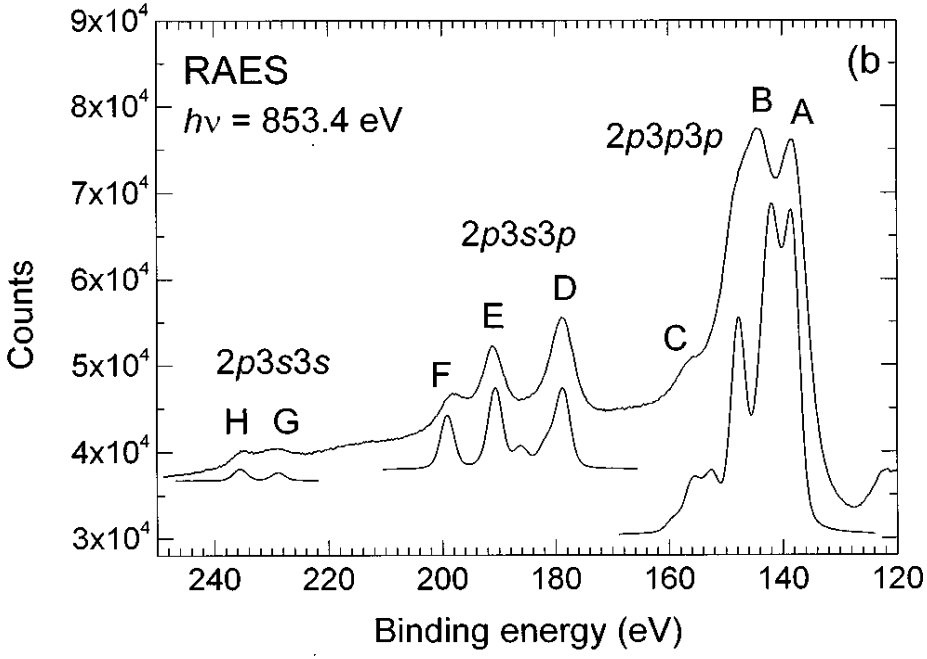
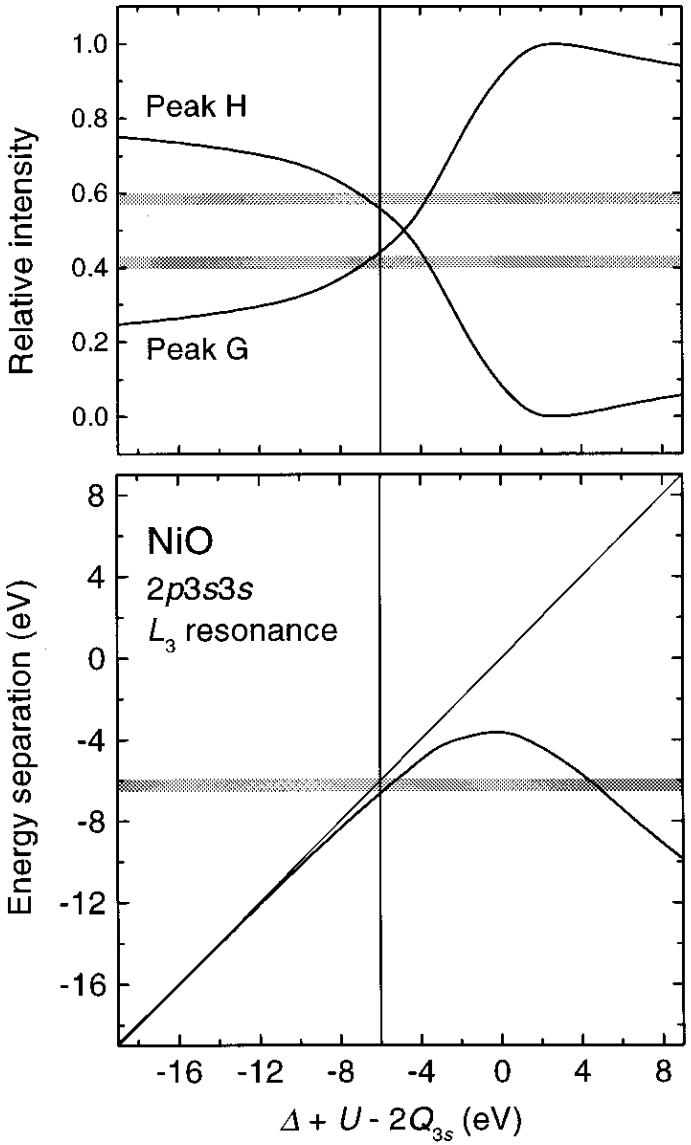
Resonant Auger of NiO







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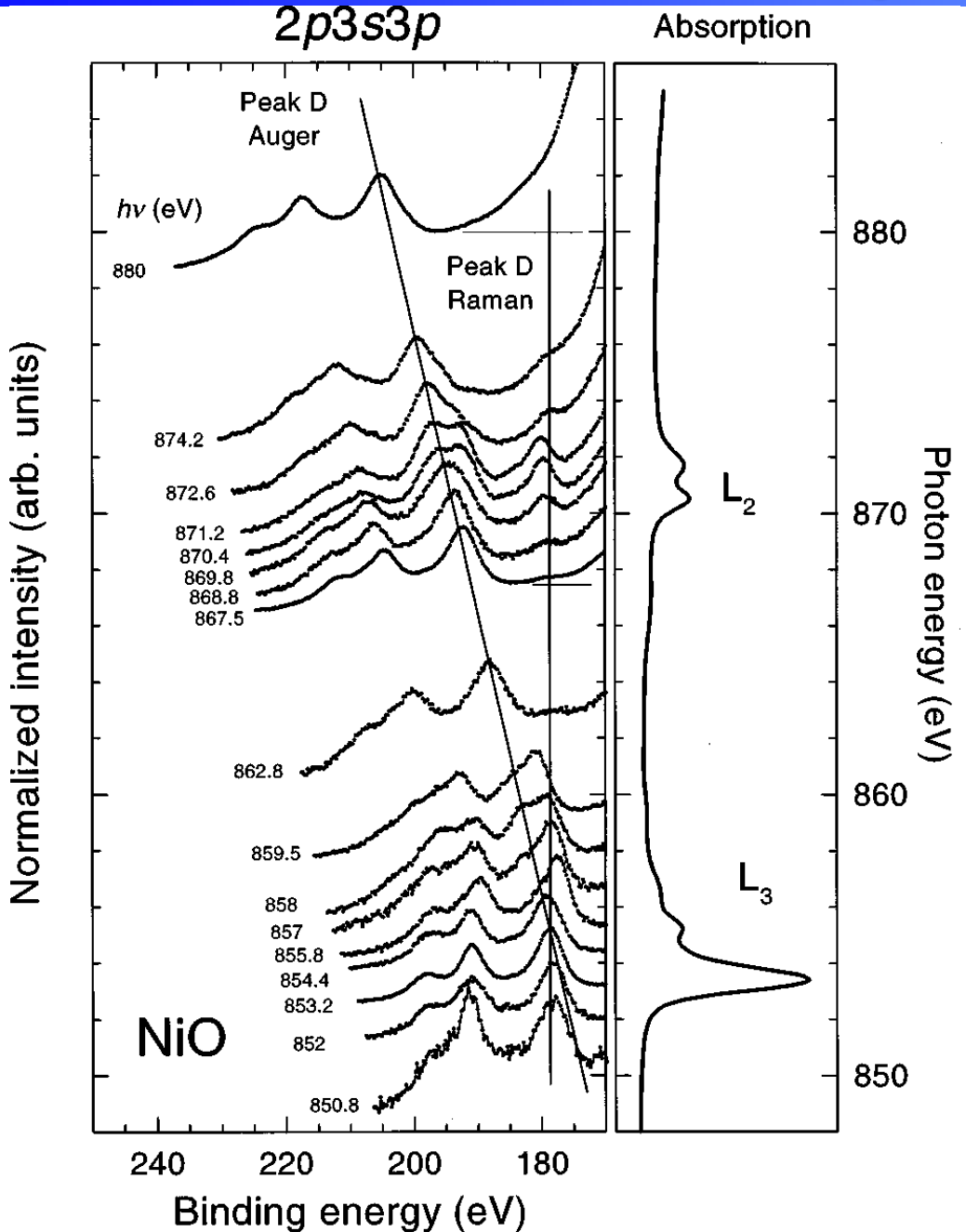
Resonant Auger of NiO



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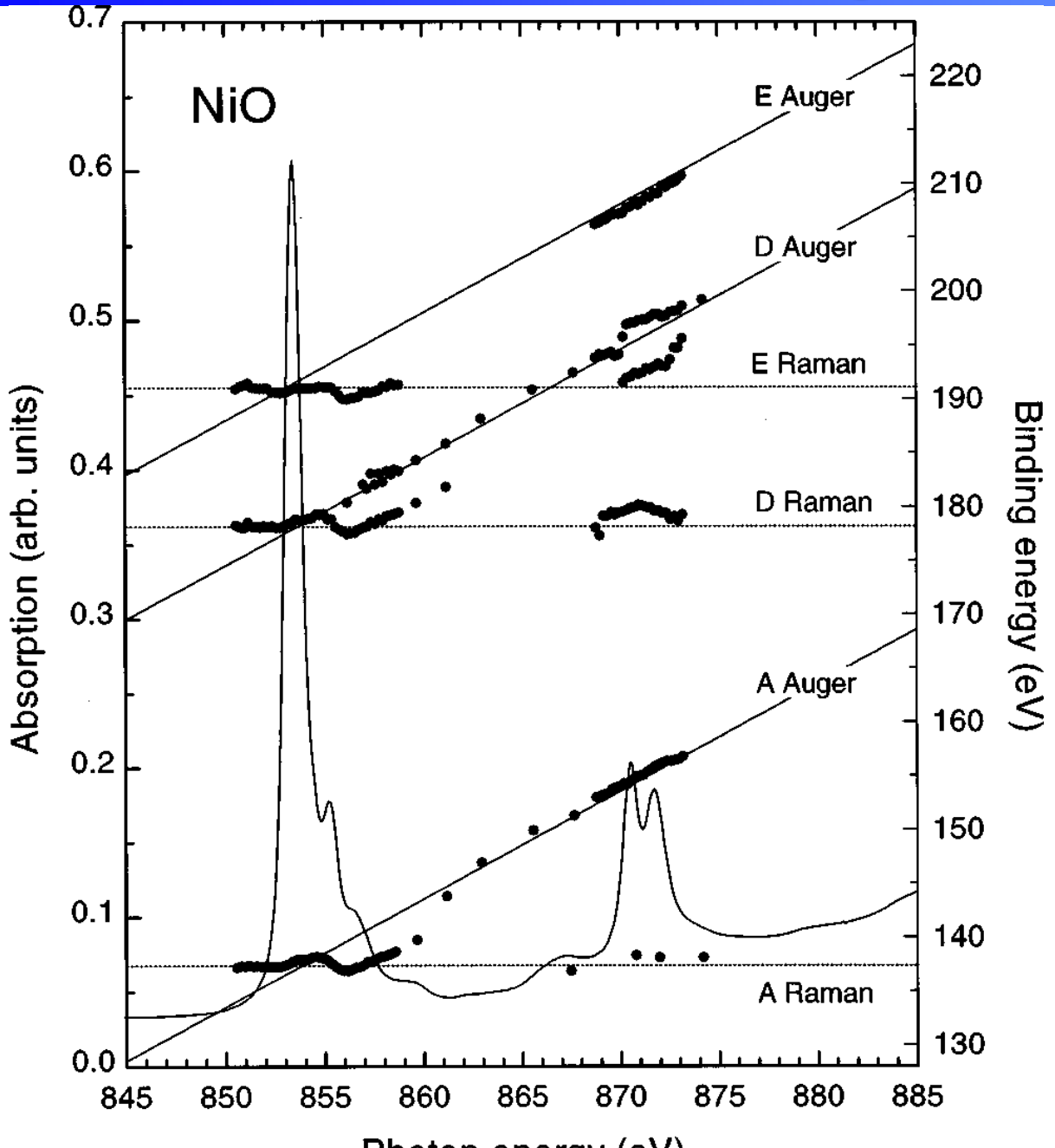
Resonant Auger of NiO



3d XPS of La2O3

3d XPS of La2O3

“La 3d XPS are due to multiplet effects”

Groot, F.M.F. de (Frank) | Thermo Scientific XPS: Kn

Veilig | https://xpssimplified.com/elements/lanthanum.php

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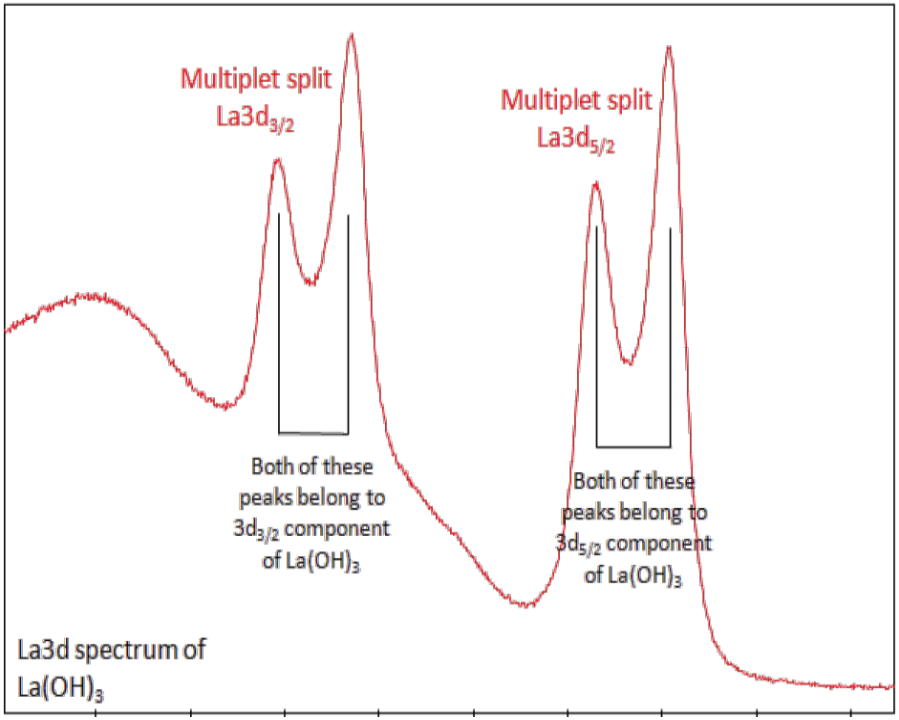
Elements

- Metalloids
- Alkali Metals
- Alkaline Earth Metals
- Transition Metals
- Other Metals
- Non-Metals
- Halogens
- Noble Gases
- Lanthanide Rare Earth
- 57 Lanthanum
- 58 Cerium
- 59 Praseodymium

Interpretation of XPS spectra

- La3d region has well separated spin-orbit components.
  - Each spin-orbit component is further split by multiplet splitting.
  - The La3d spectrum from a pure $La(OH)_3$ sample, for example, will have four visible components, even though there is only one chemical state.



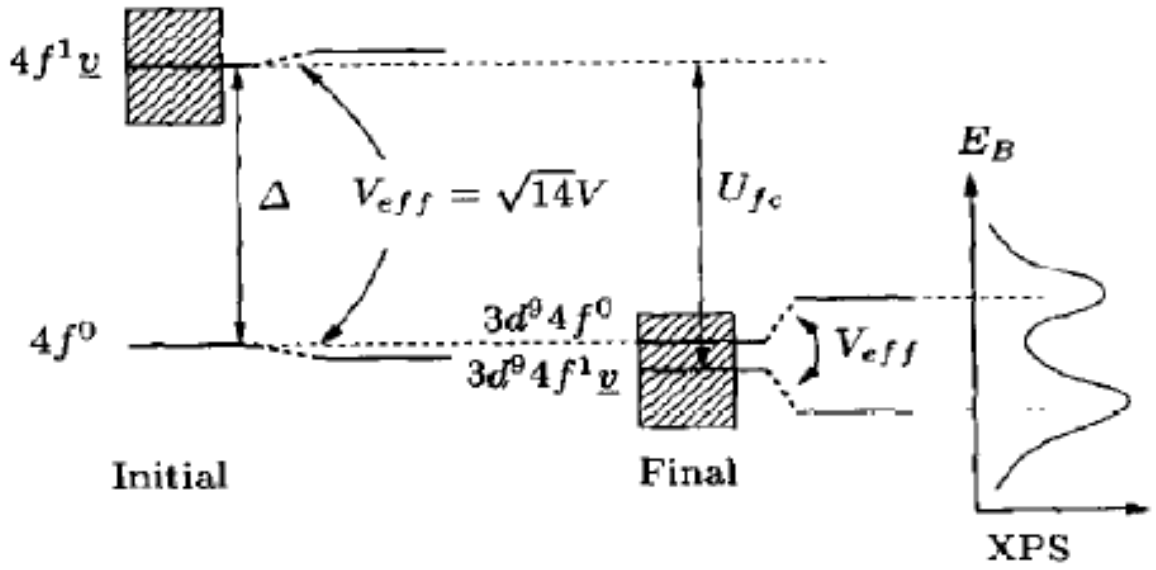
3d XPS of La2O3

"La 3d XPS are due to multiplet effects?"

4f0 transition to $3d^9\ 4f^0$ + e,
so there are NO multiplets (no e-e interactions)

3d XPS of La2O3

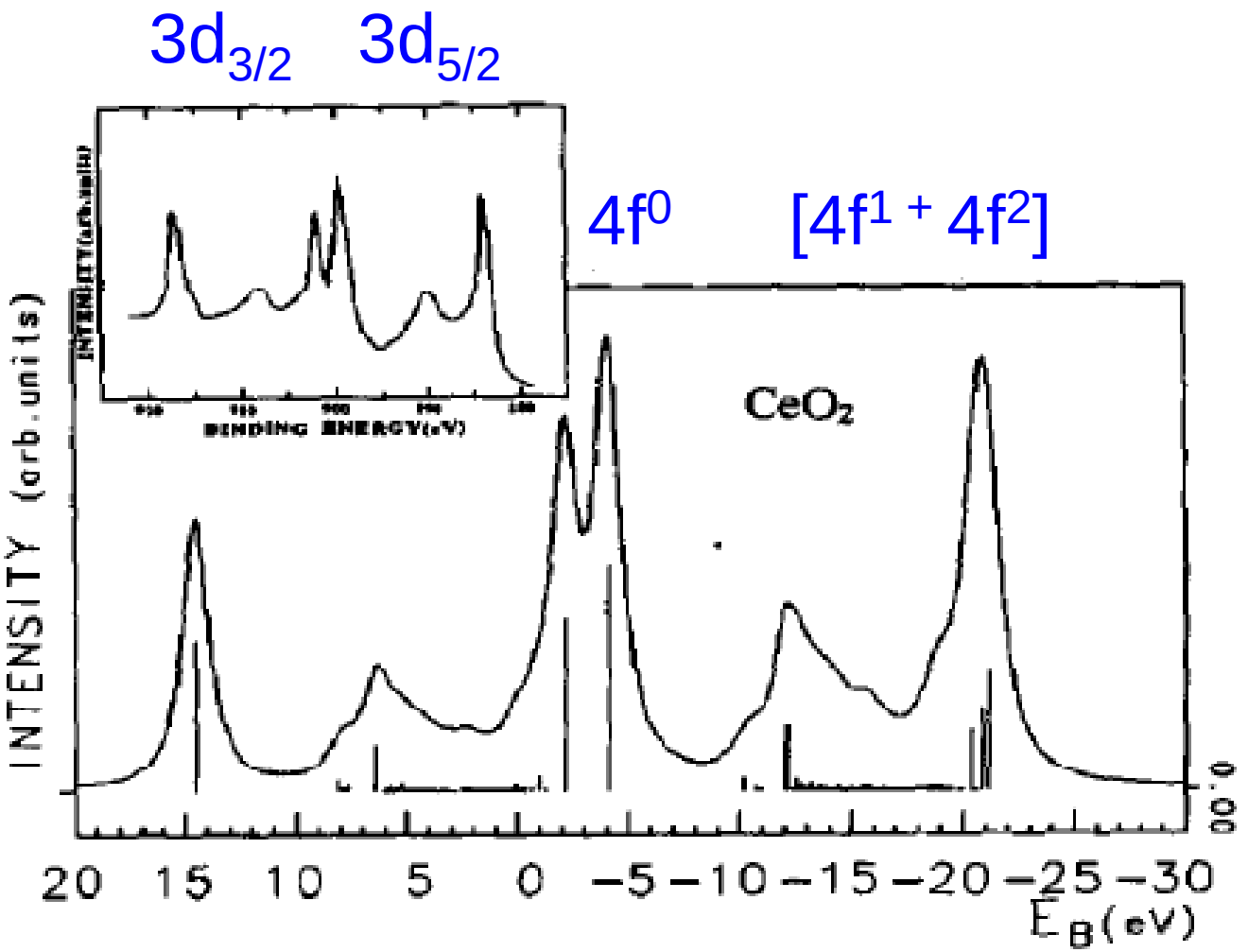
"La 3d XPS are due to multiplet effects?"



Explanation by Kotani's group: J. Elec. Spec. 60, 257 (1992)

Peaks split due to **charge transfer effect**

3d XPS of CeO2



J. Elec. Spec. 60, 257 (1992)