Applications of RIXS in Catalysis and Magnetism

- X-ray Absorption Spectroscopy (XAS)
- Resonant Inelastic X-ray Scattering (RIXS)

- Soft x-ray Spectra with Hard X-rays
- Valence Selective XAS
- Spectral Sharpening

- Application to Catalysis: FeZSM5
- Application to Magnetic Materials

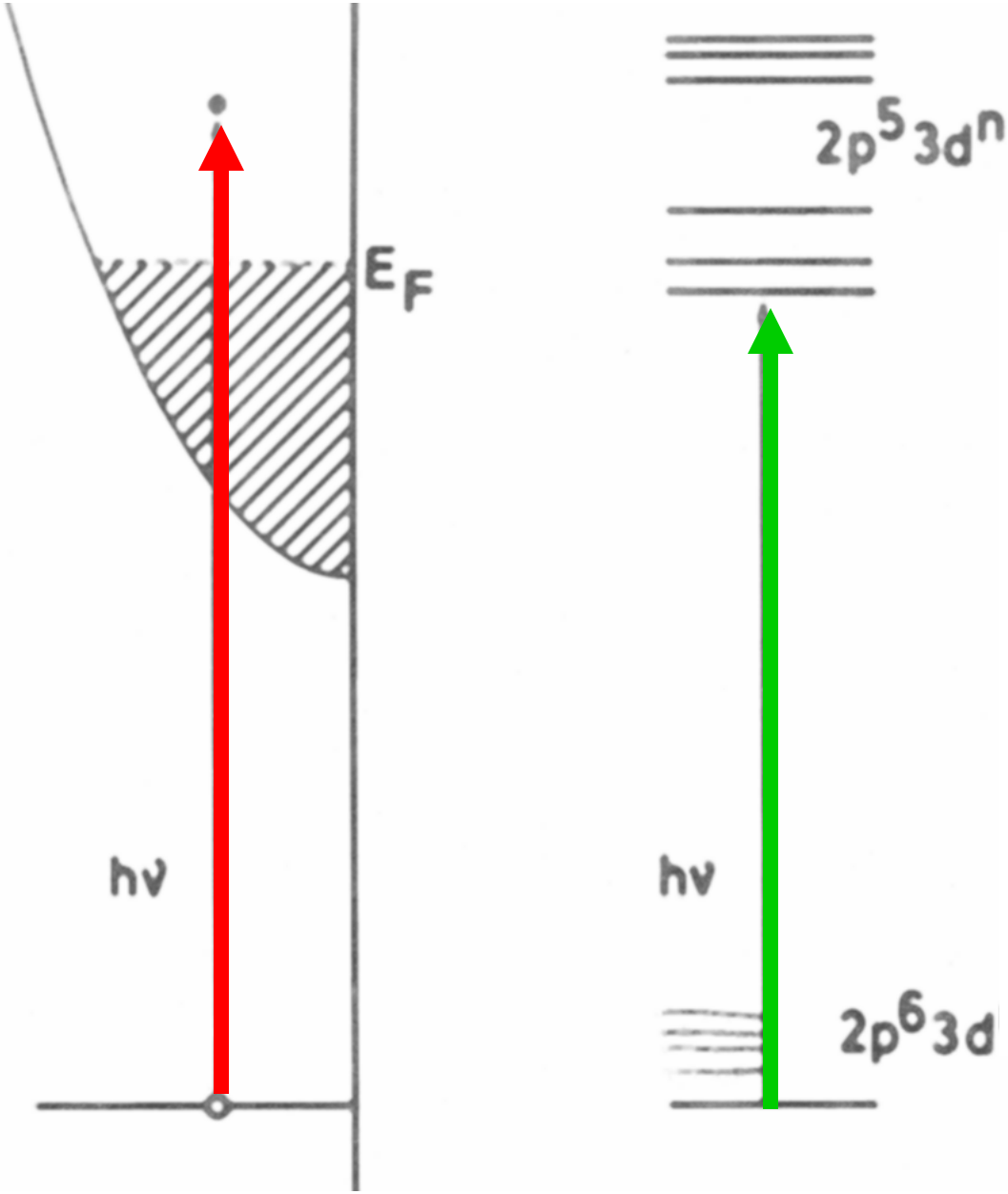
Applications of RIXS in Catalysis and Magnetism

- **Acknowledgements**

- **Pieter Glatzel**

- Uwe Bergmann, Steve Cramer, Erik Wasinger, Ed Solomon, Wolfgang Caliebe, Chi-chang Kao, Willem Heijboer, Axel Knop-Gericke, Michael Krisch.

X-ray Absorption Spectroscopy



Single Particle:

1s edges

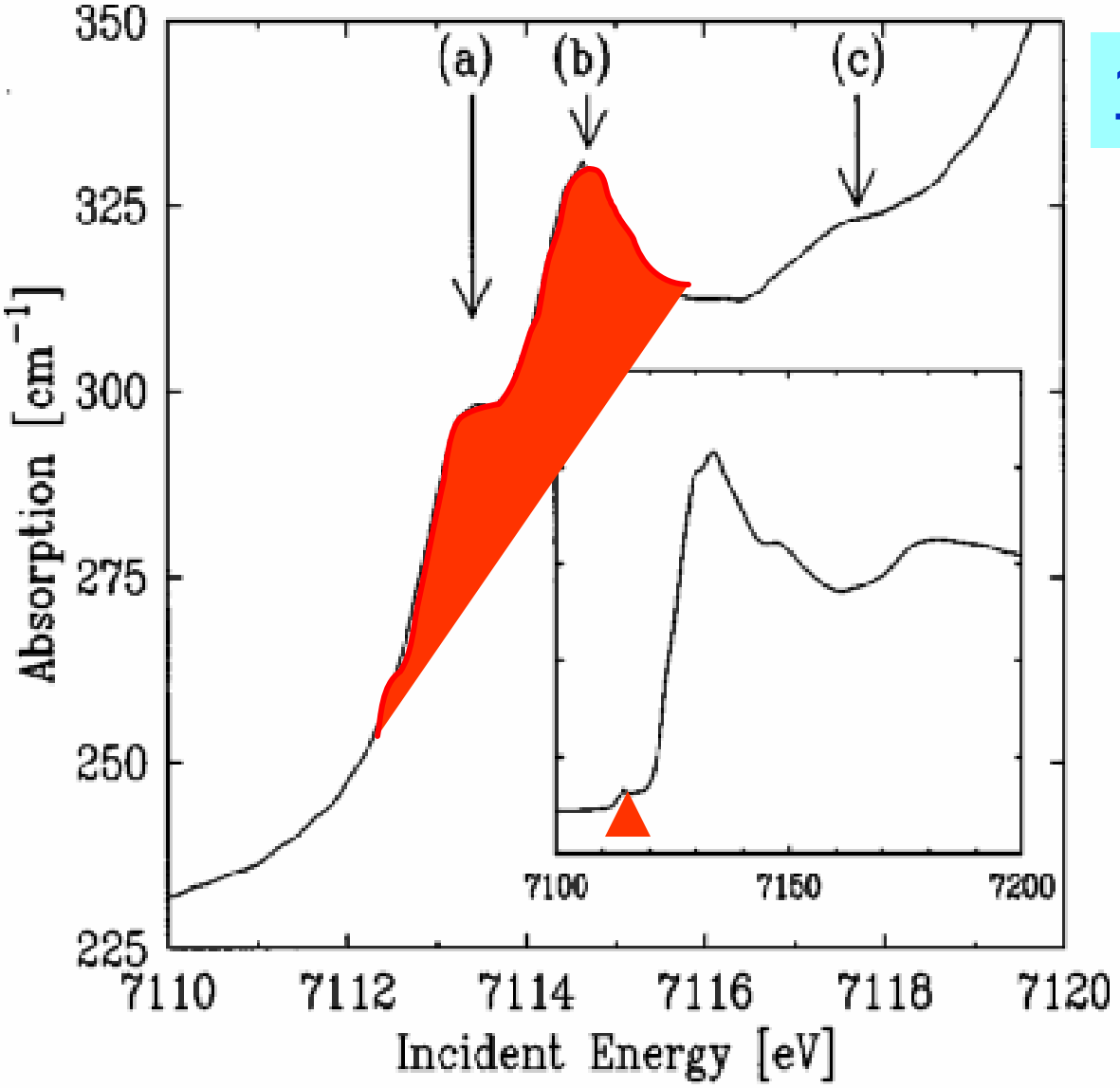
Hard x-rays

Multiplets:

2p, 3s, 3p edges

Soft x-rays

Resonant Inelastic X-ray Scattering



1s XAS of Fe_2O_3

K edge:

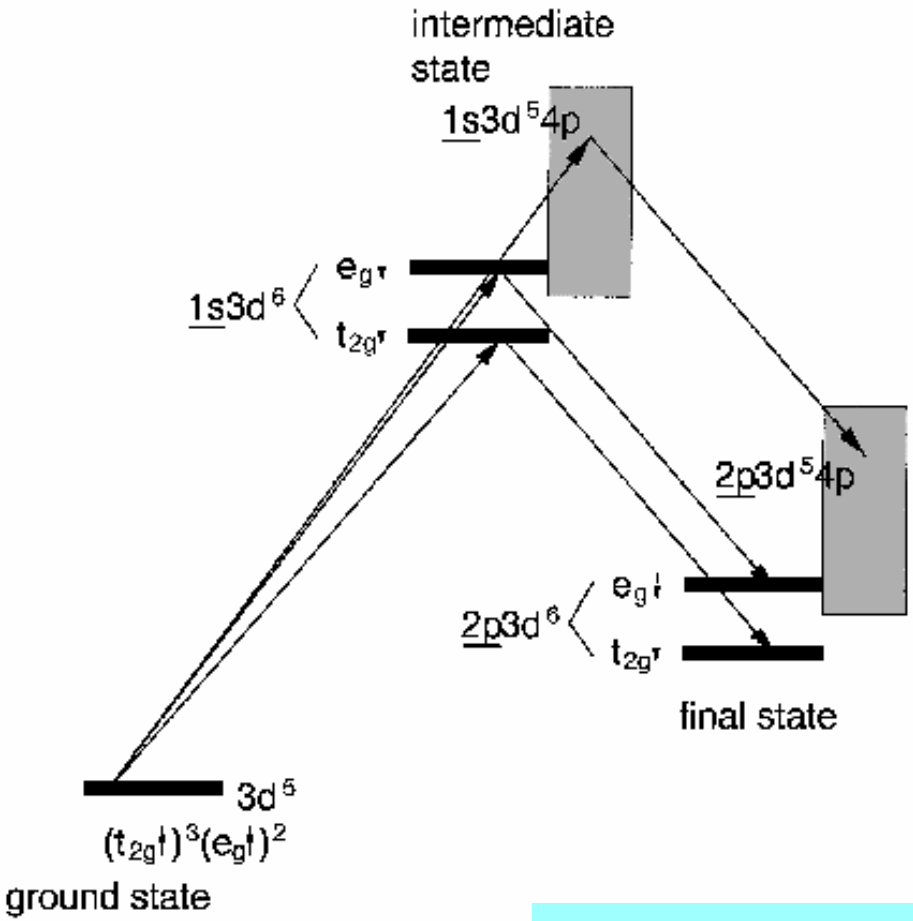
1s to 4p

Pre-edge:

1s to 3d

Phys. Rev. B. 58, 13452 (1998)

Resonant Inelastic X-ray Scattering



1s2p RIXS of Fe_2O_3

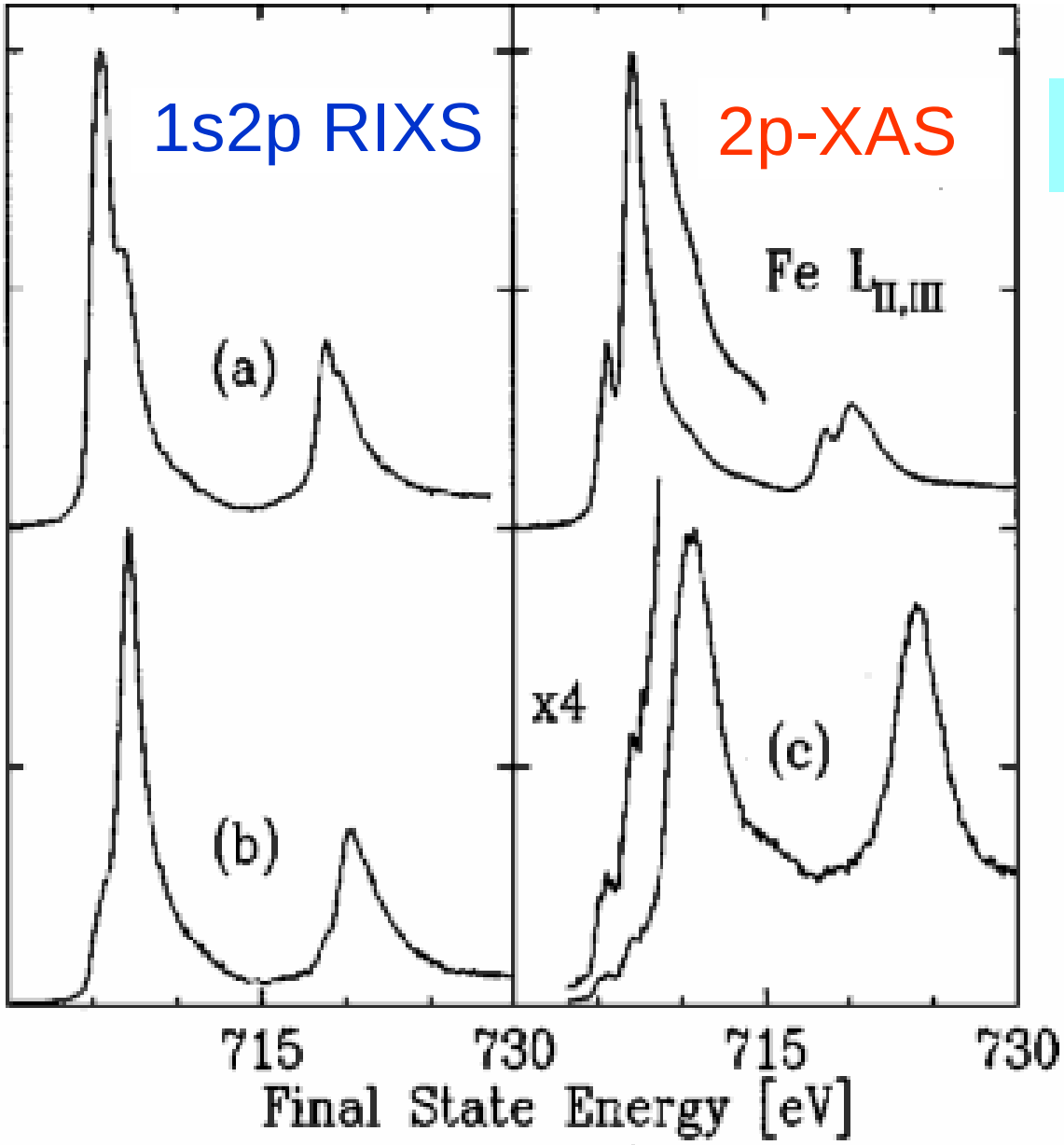
Quadrupole to 3d-states

Dipole to 4p-states

Decay of 2p-electron into 1s-hole

Final state identical to 2p XAS

Resonant Inelastic X-ray Scattering

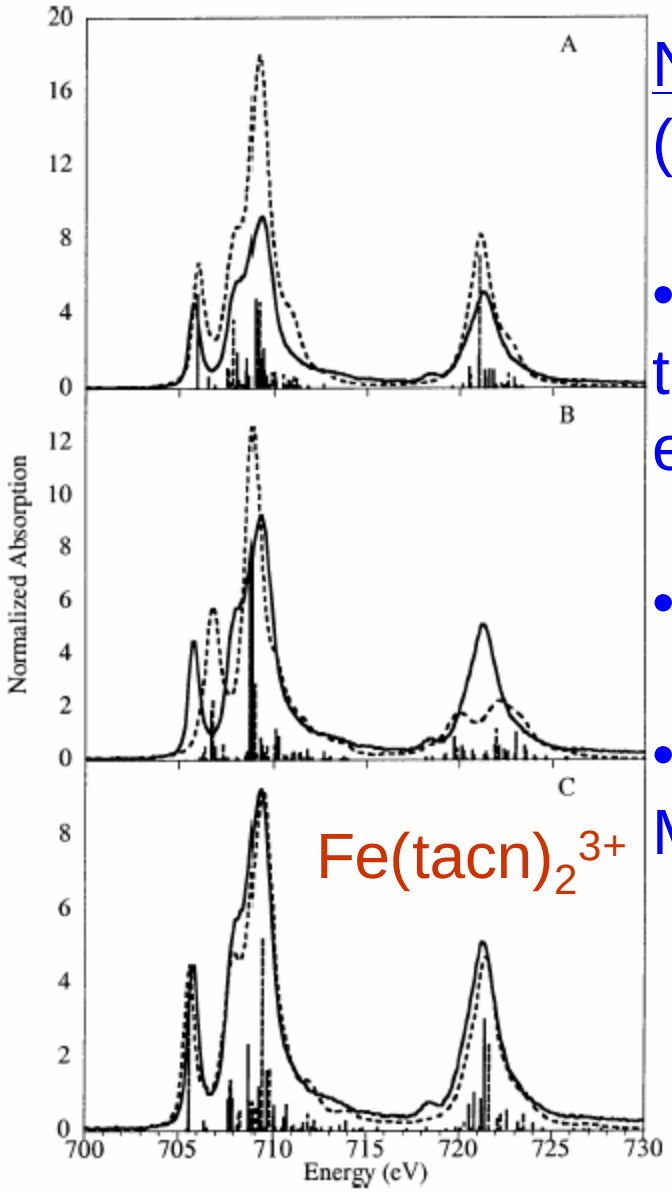


1s2p RIXS of Fe_2O_3

'soft x-ray spectra with hard x-rays'

Phys. Rev. B. 58, 13452 (1998)

Soft X-ray absorption

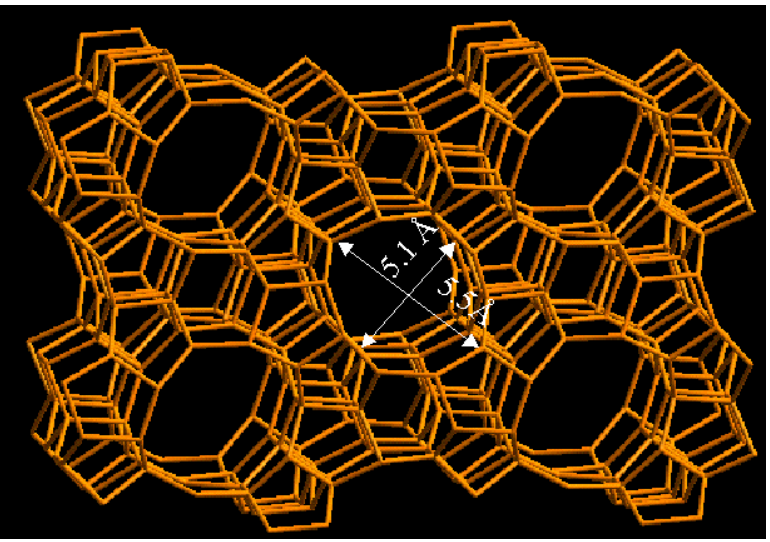


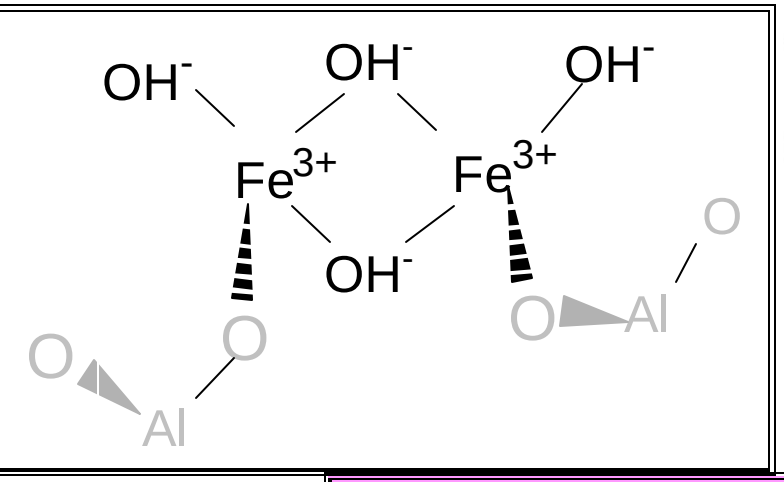
New developments:
(with Erik Wasinger, Ed Solomon)

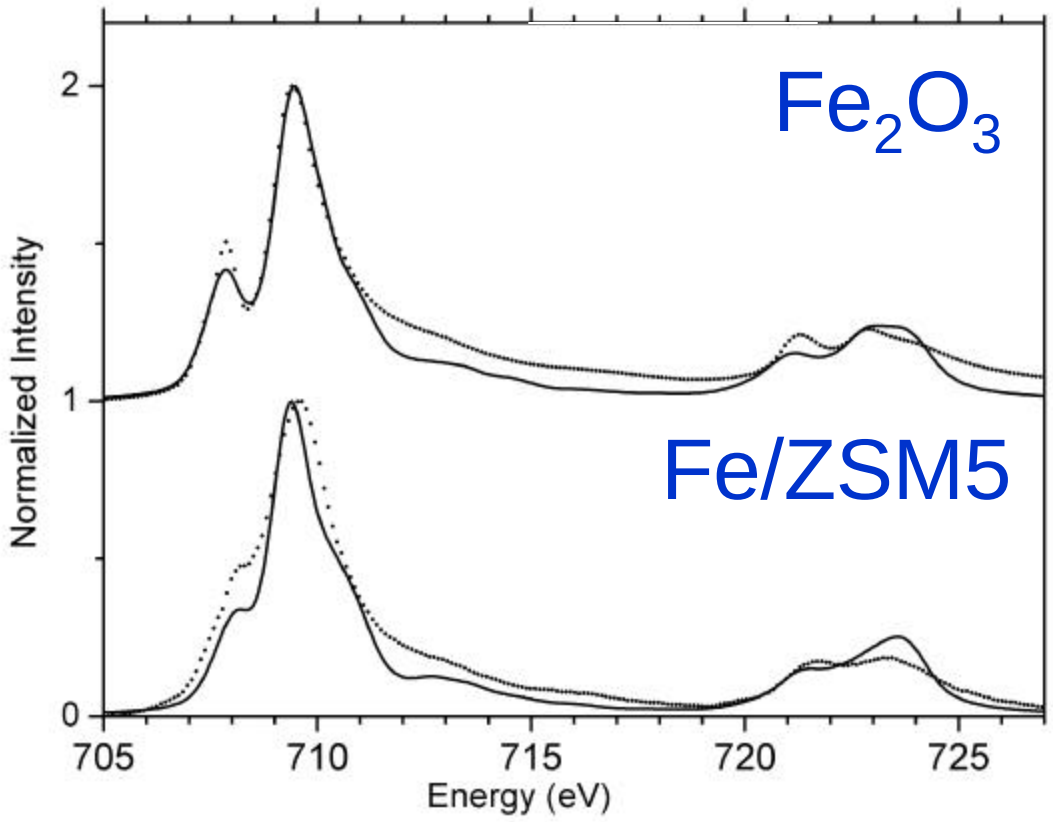
- Projection of charge transfer simulation to 'constituents', for example $3d^5$-t_{2g}, $3d^5$-e_g, $3d^6\underline{L}$-t_{2g} and $3d^6\underline{L}$-e_g, >> DOC
- Projection to lower symmetries and spin.
- Inclusion of σ and π bonding and of MLCT (next to LMCT)

JACS (2003)

Application to Catalysis: Fe/ZSM5

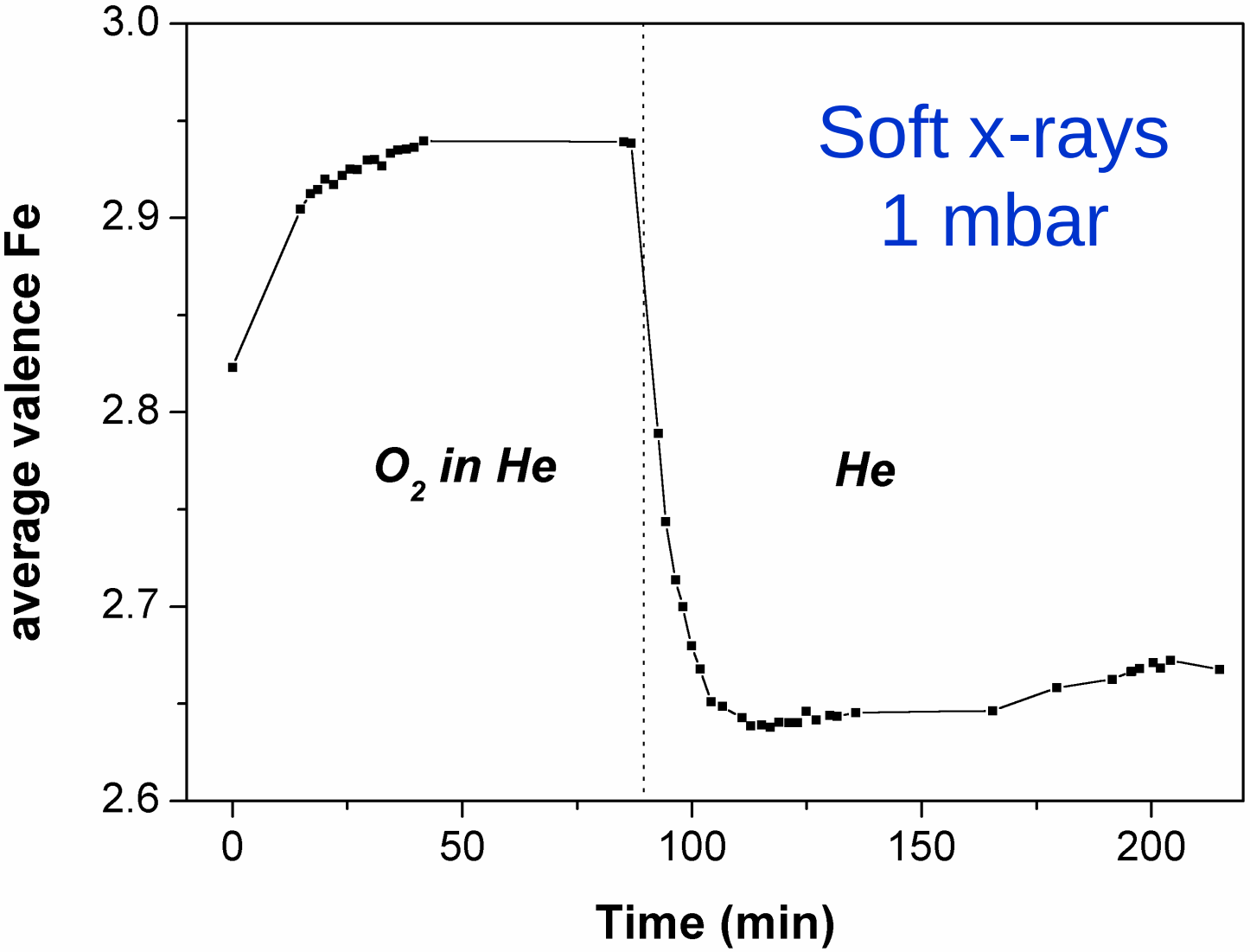






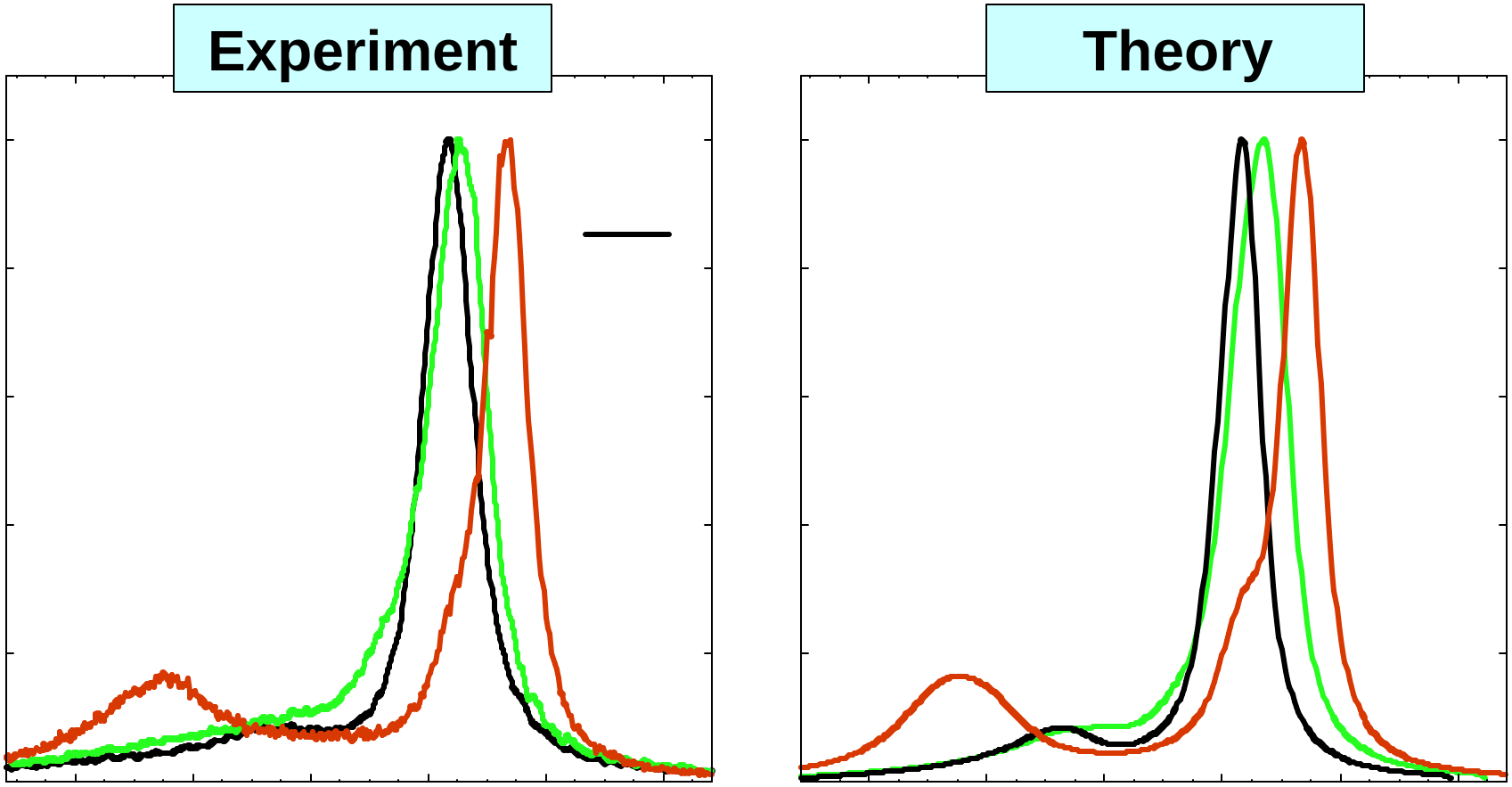
J. Phys. Chem. B. (in press)
Phys. Chem. Chem. Phys. 5, 4484 (2003)

Application to Catalysis: Fe/ZSM5



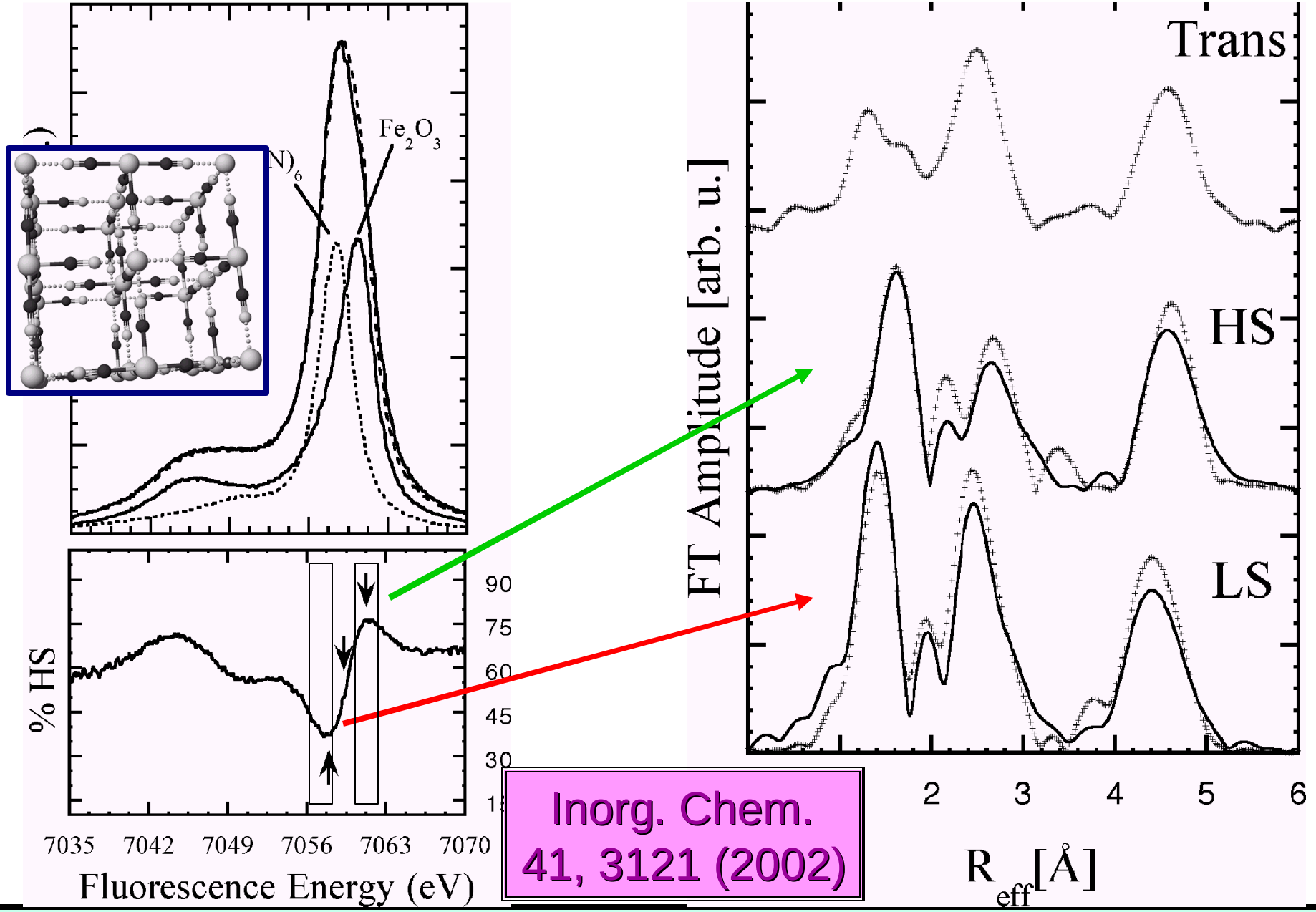
Valence shifts in X-ray Emission

Chemical Dependence of Kβ Emission



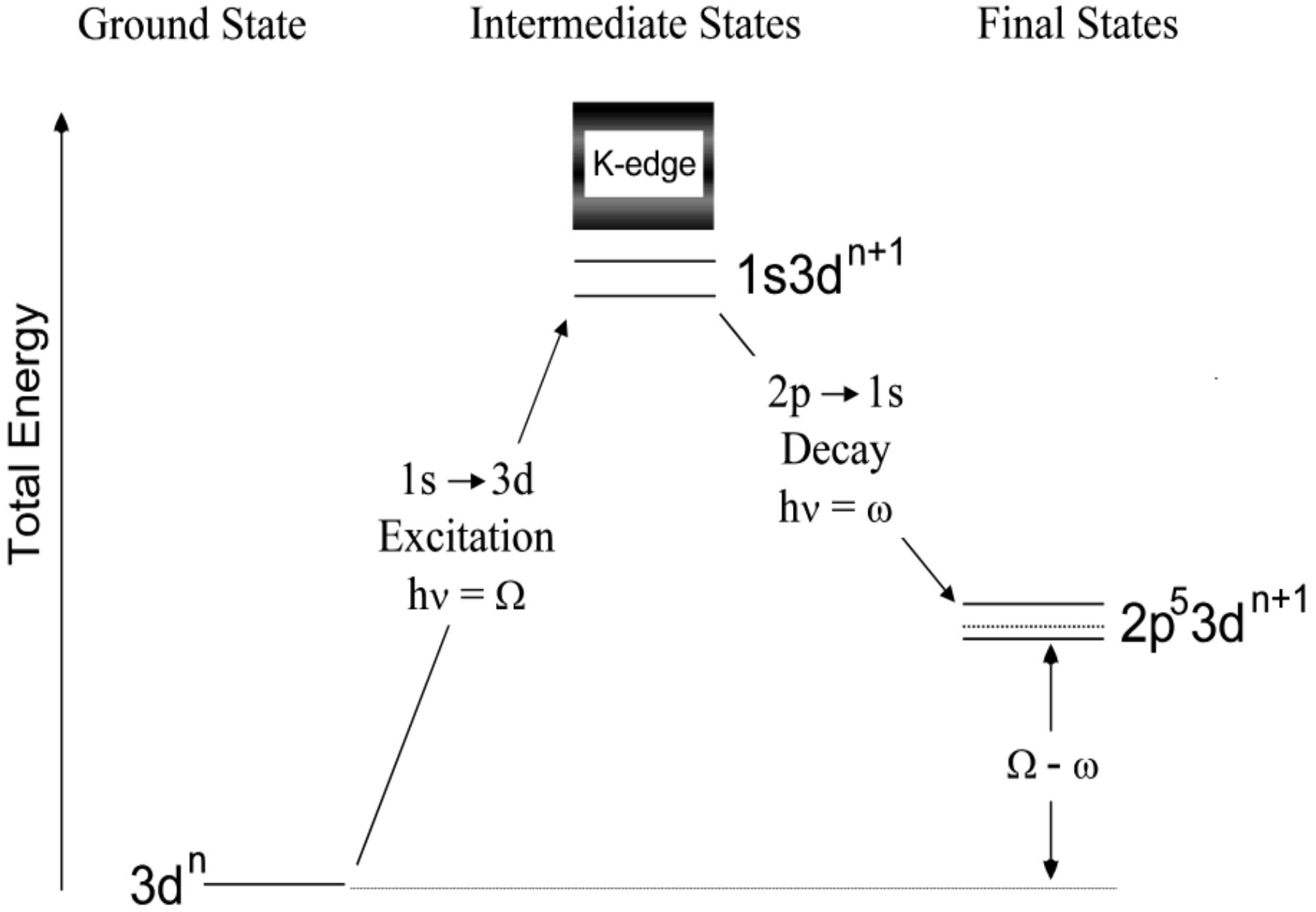
Equal center-of-gravity energies used in calculations!

Valence selective XAS

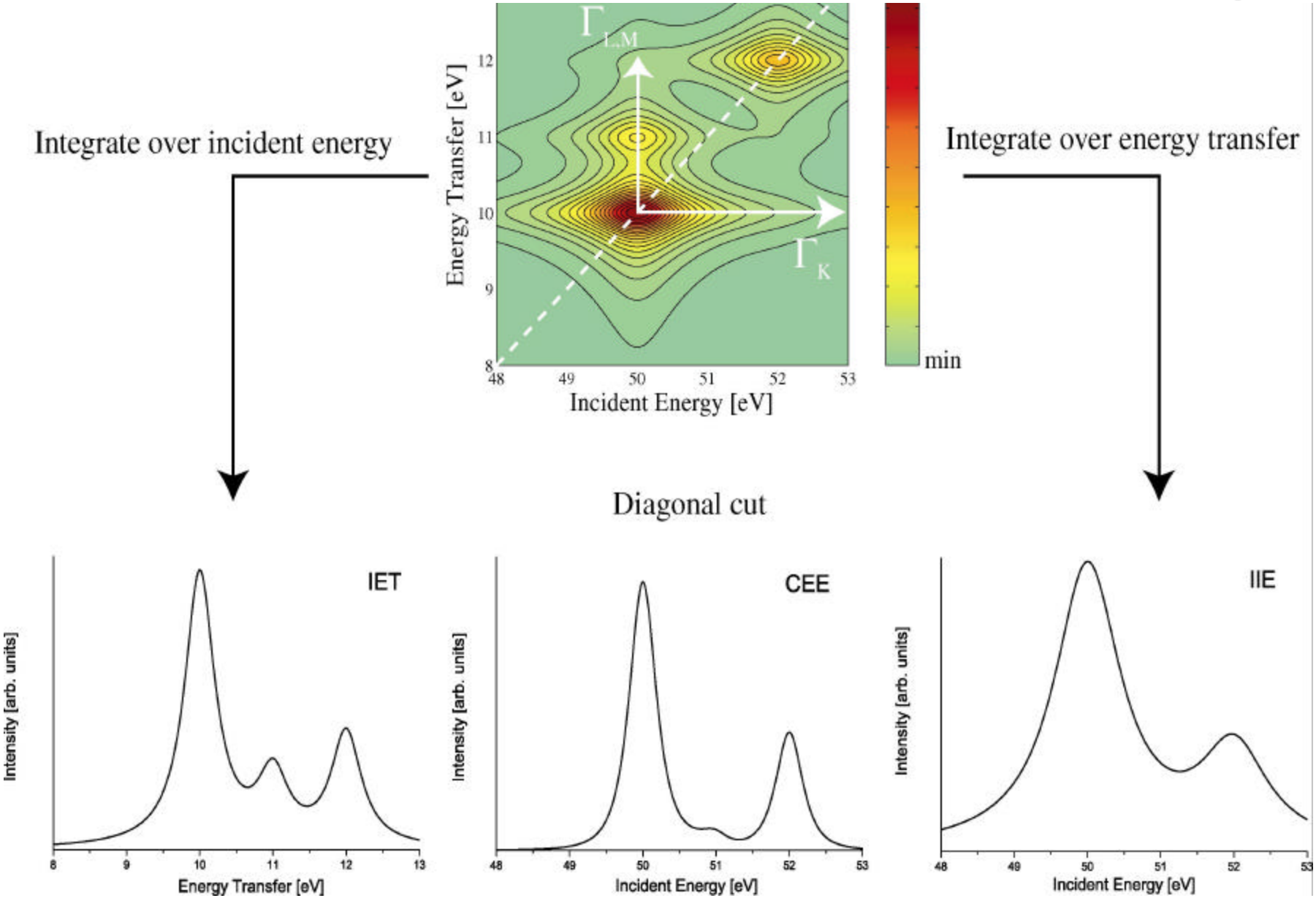


Inorg. Chem.
41, 3121 (2002)

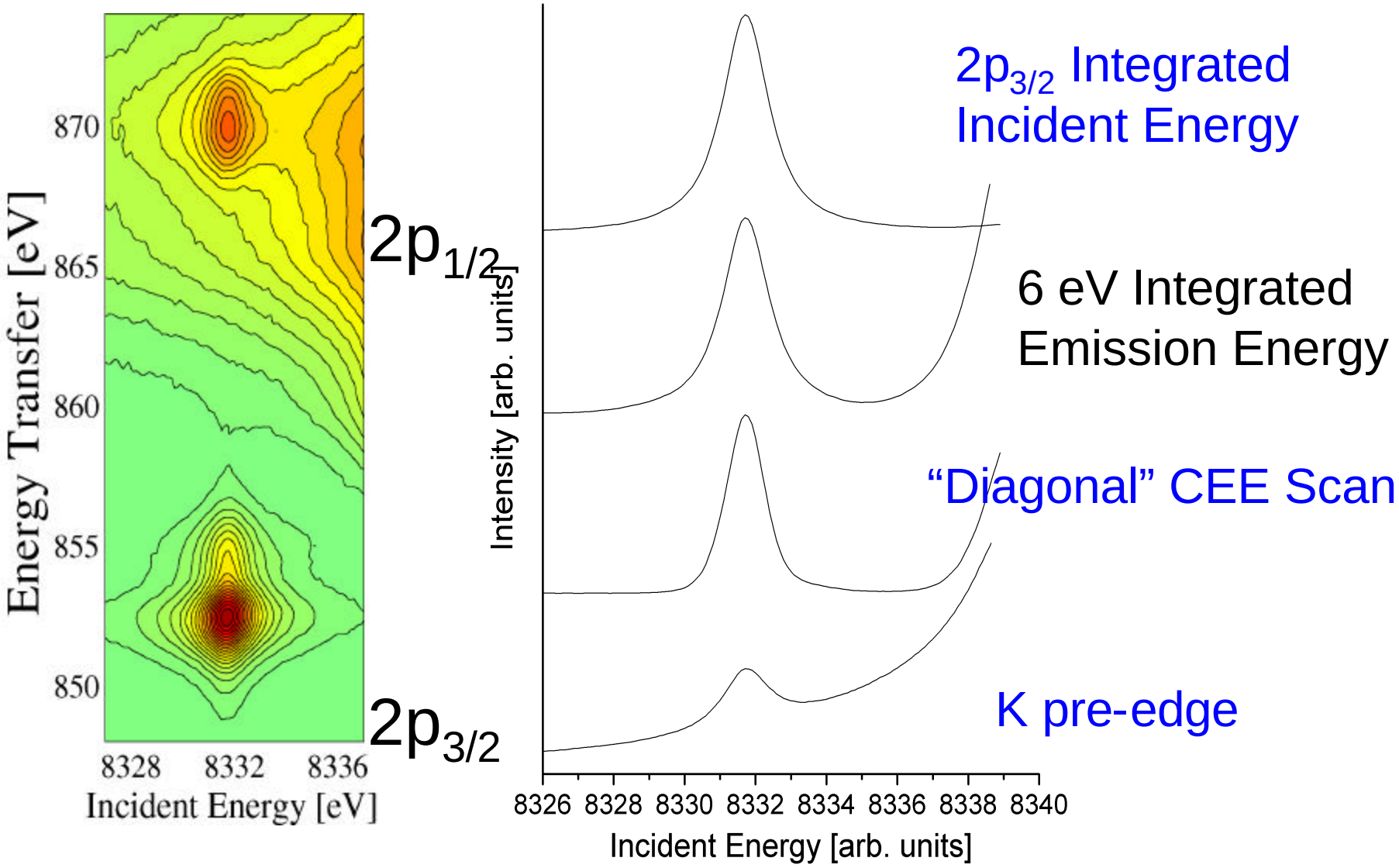
Resonant Inelastic X-ray Scattering



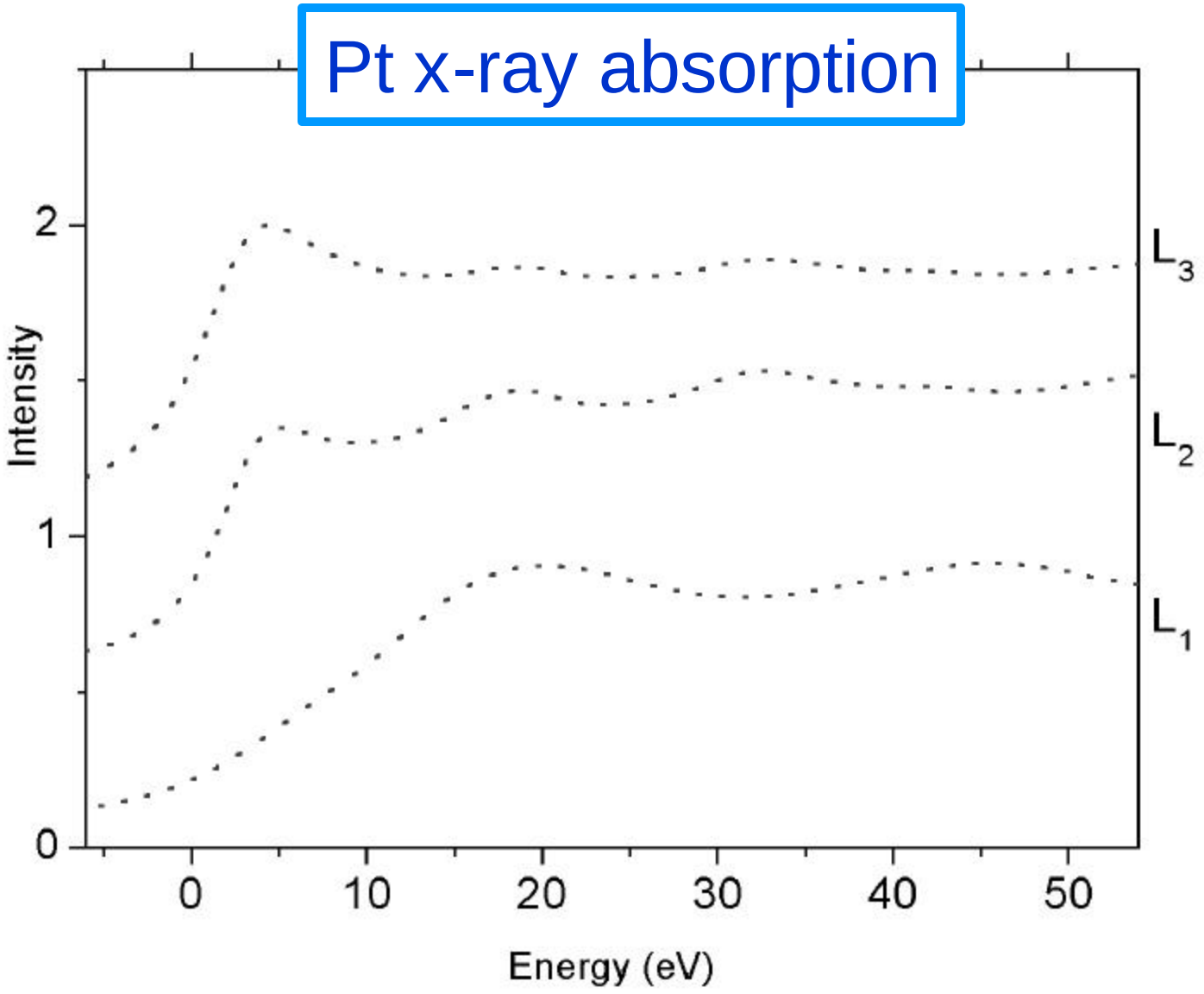
Resonant Inelastic X-ray Scattering



Spectral Sharpening

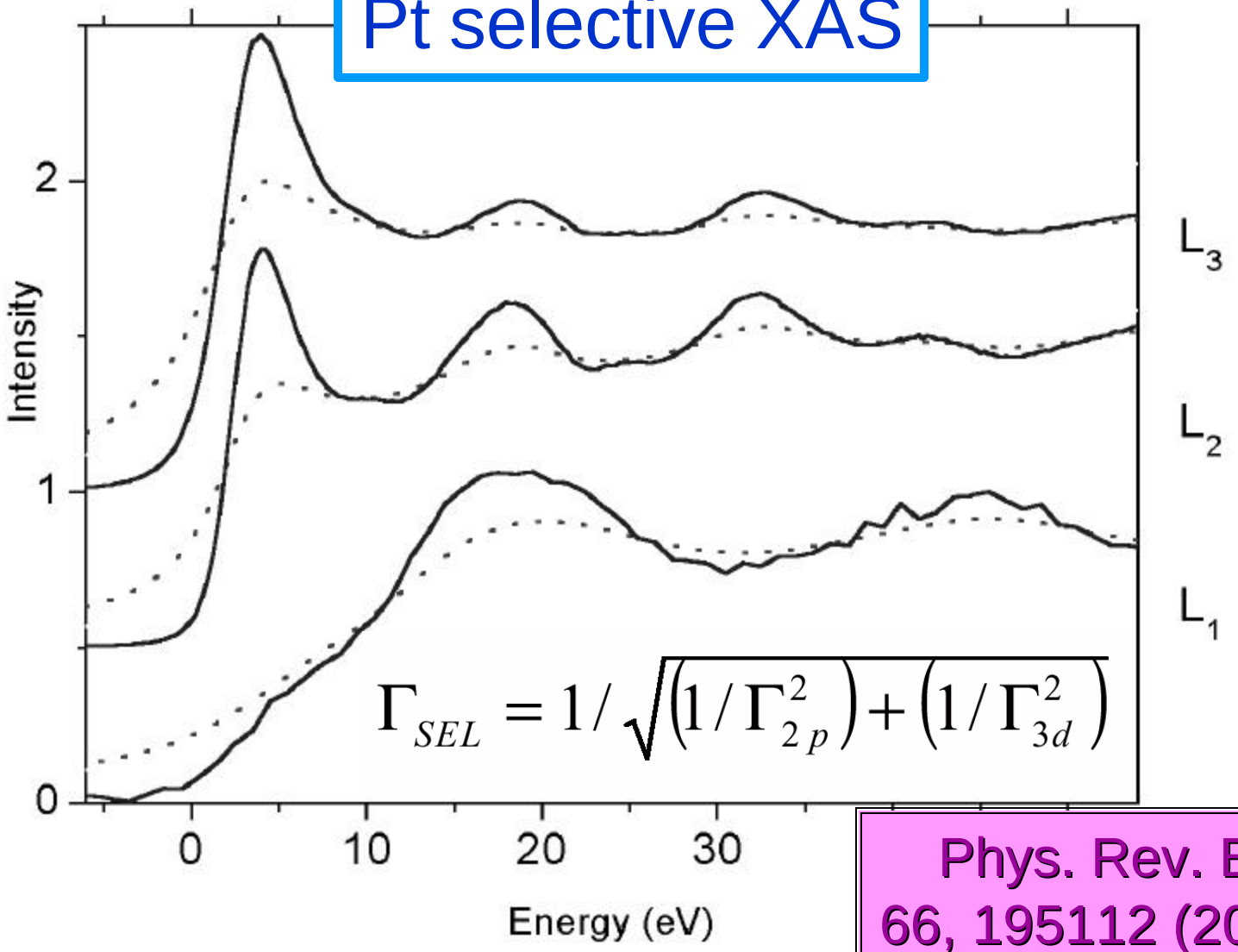


Spectral Sharpening



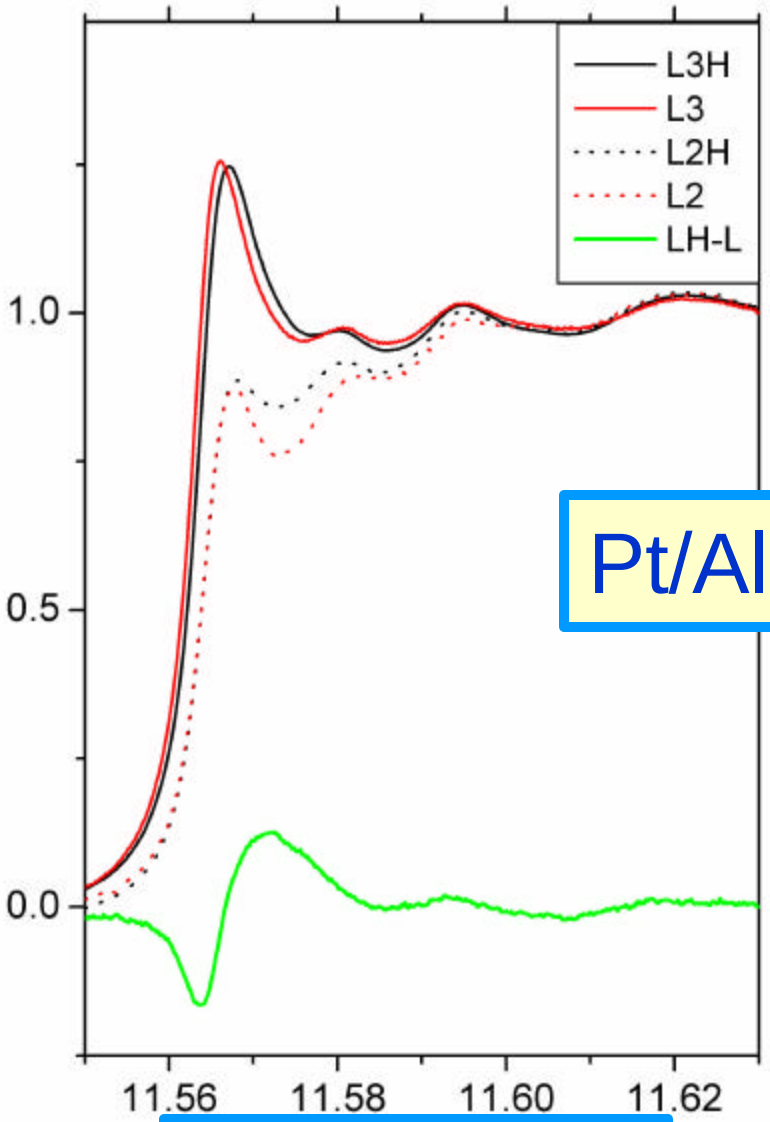
Spectral Sharpening

Pt selective XAS

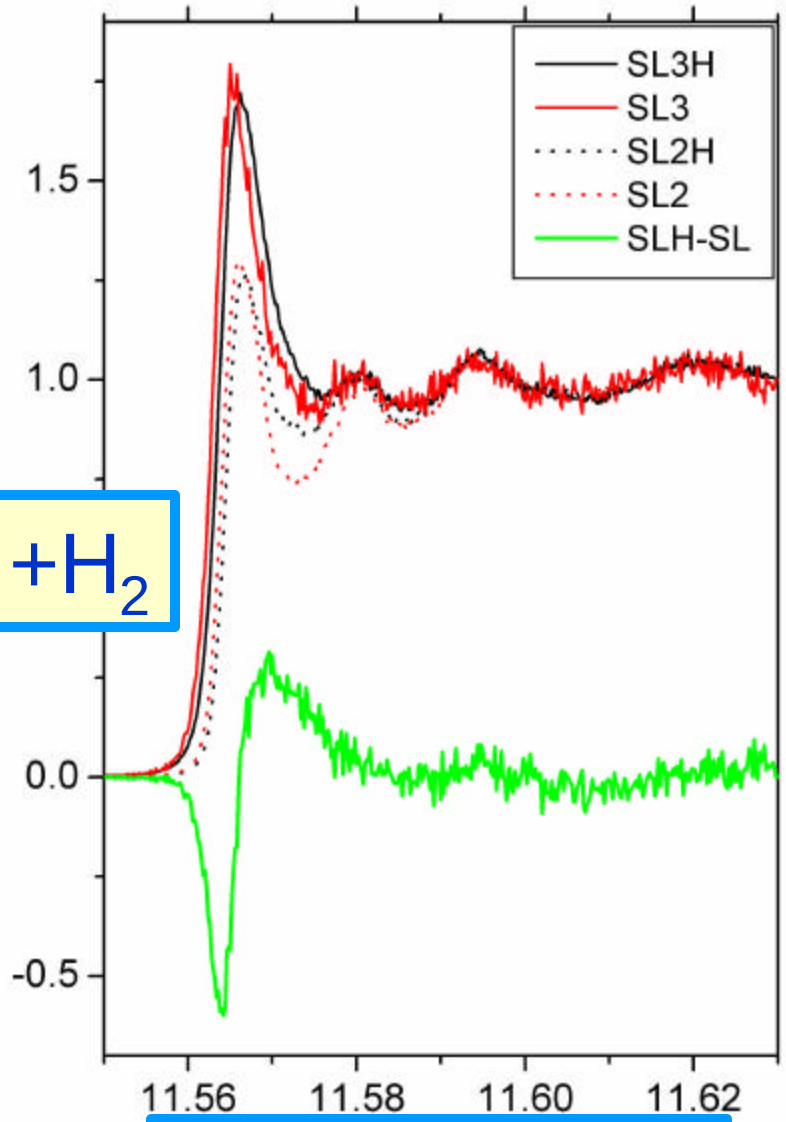


Phys. Rev. B. 66, 195112 (2002)

Spectral Sharpening



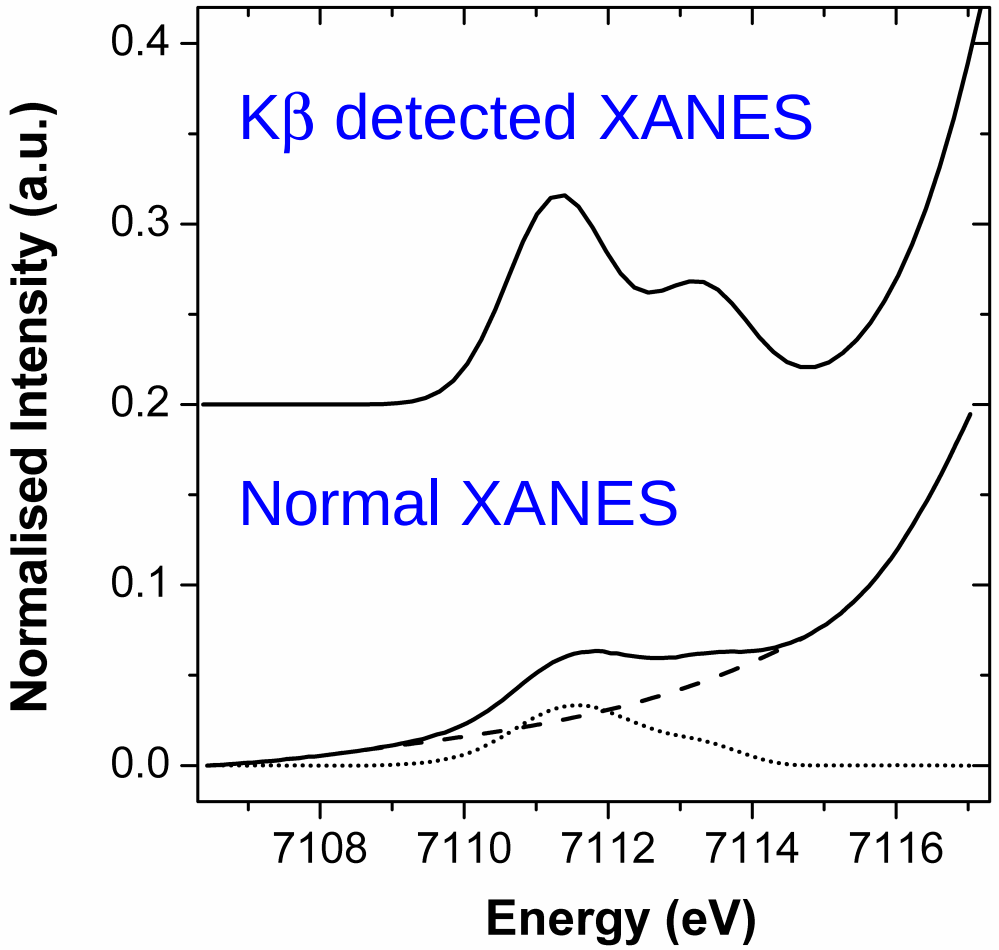
$Pt/Al_2O_3 + H_2$

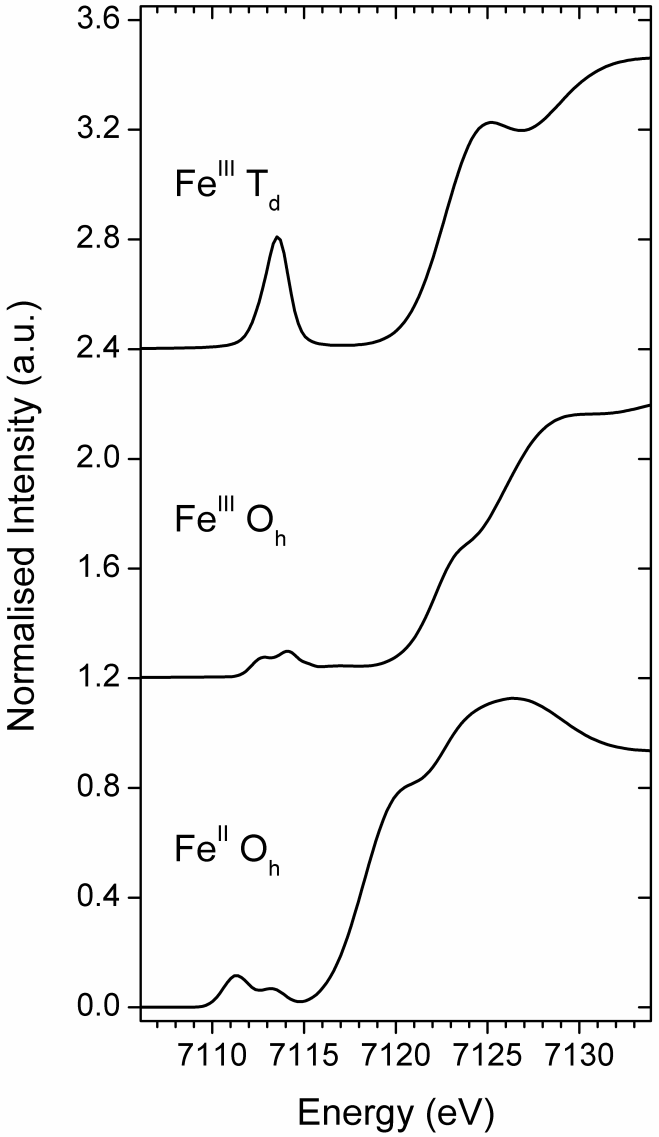


normal XAS

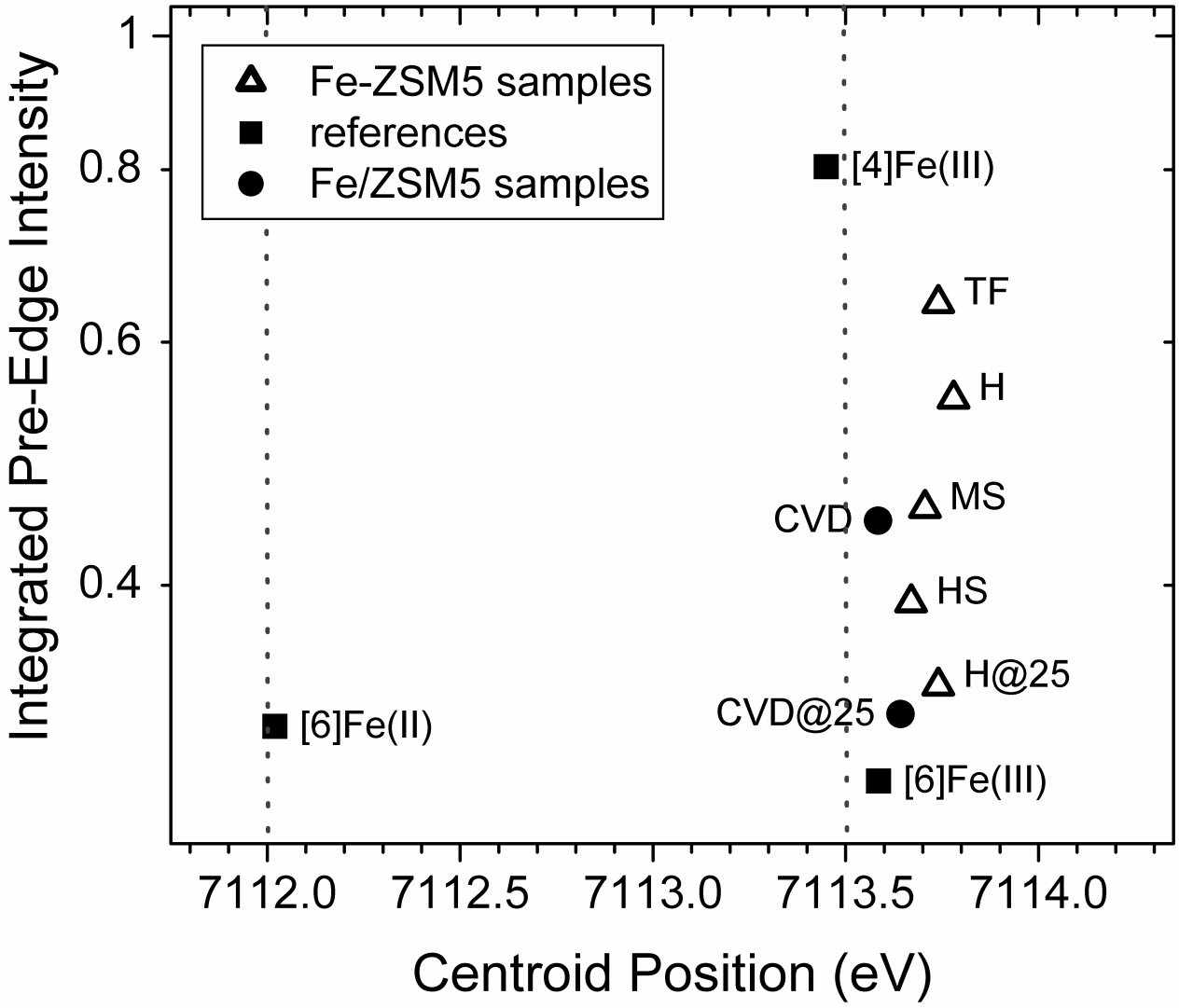
selective XAS

Application to Catalysis: Fe/ZSM5



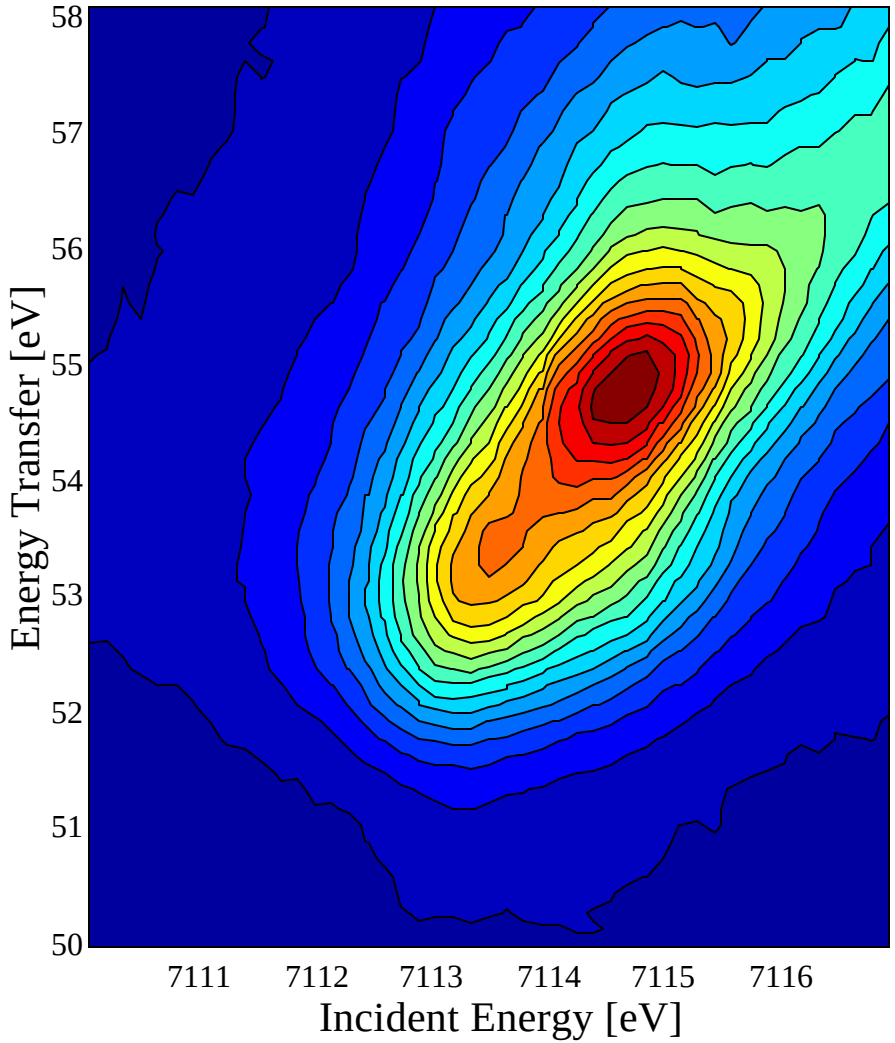


Application to Catalysis: Fe/ZSM5



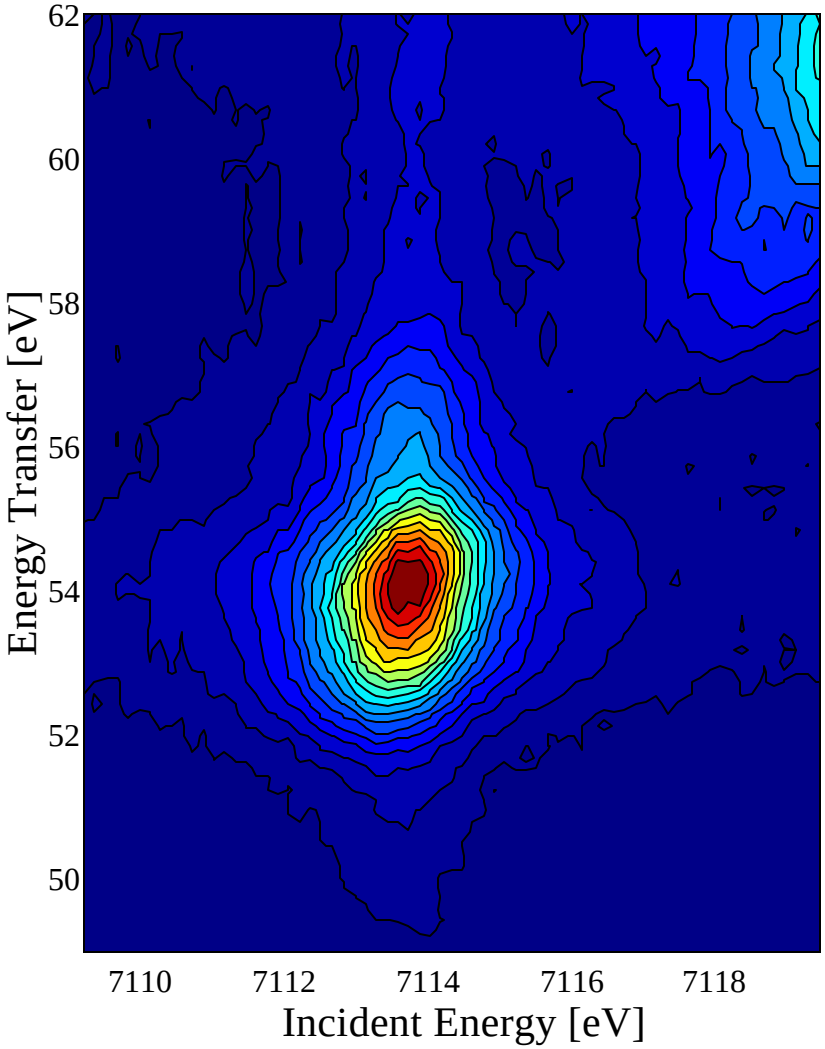
RIXS of Iron compounds

Fe^{3+} in Fe_2O_3

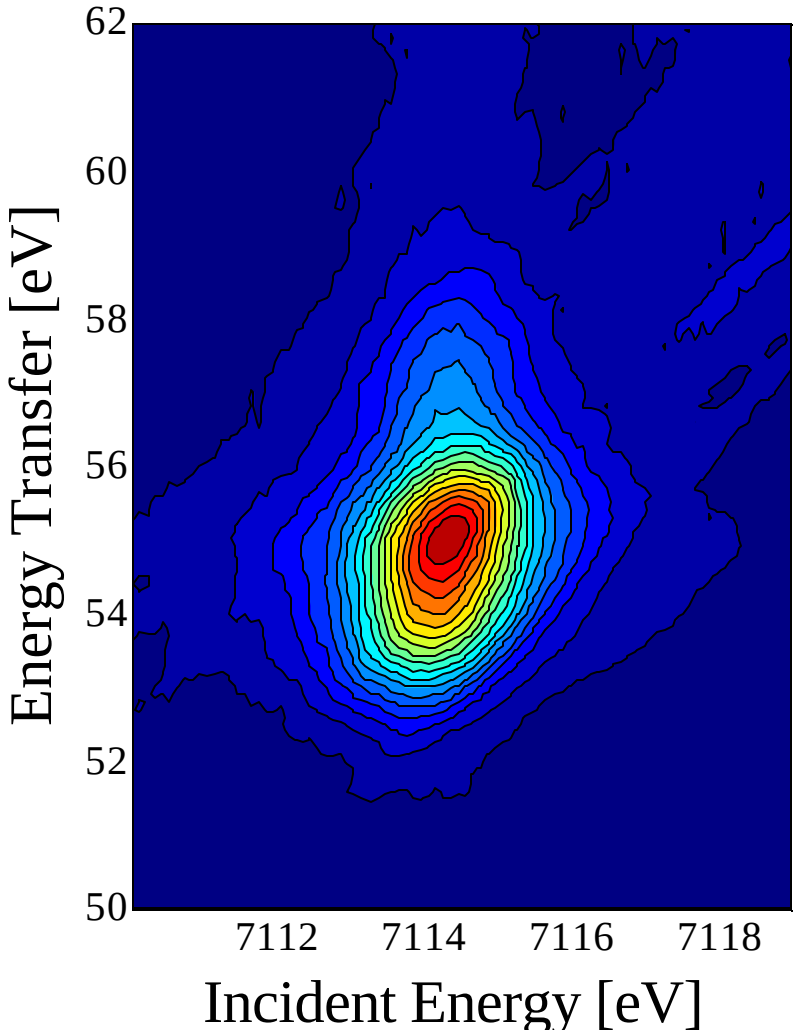


RIXS of Iron compounds

Fe^{3+} in $[FeCl_4]^{1-}$ Td

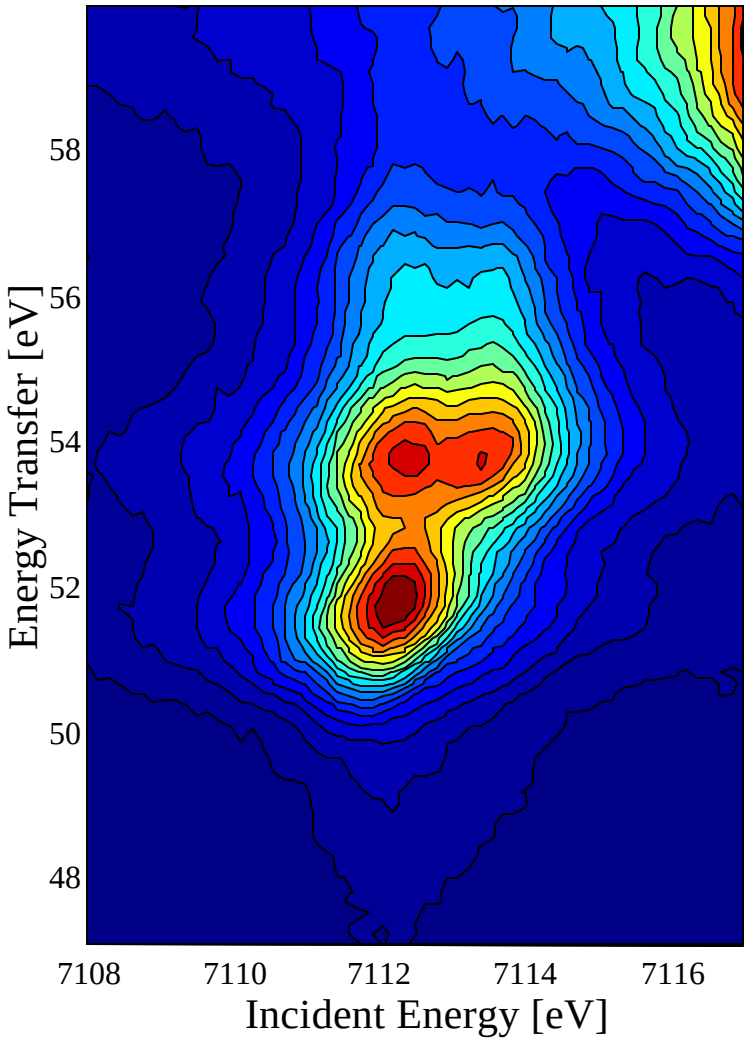


Fe^{3+} Phosphate Td

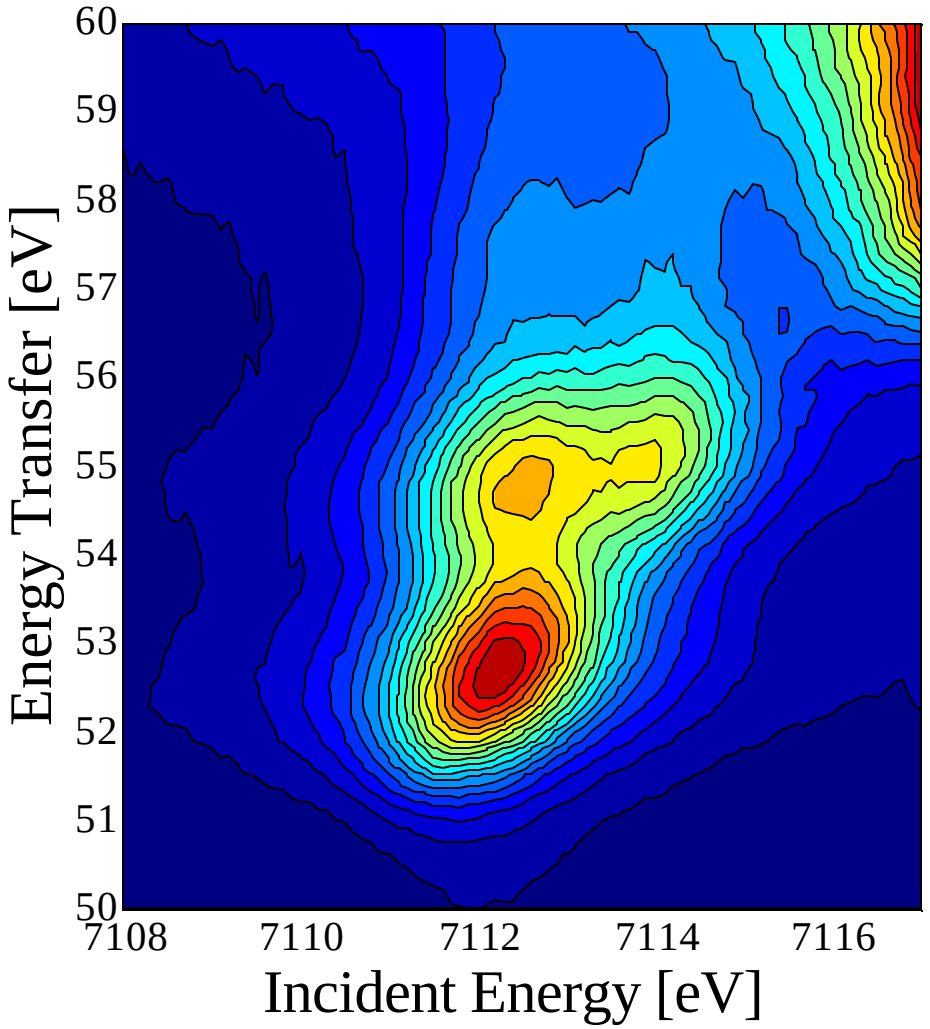


RIXS of Iron compounds

Fe^{2+} in $[FeCl_4]^{2-}$ T_d

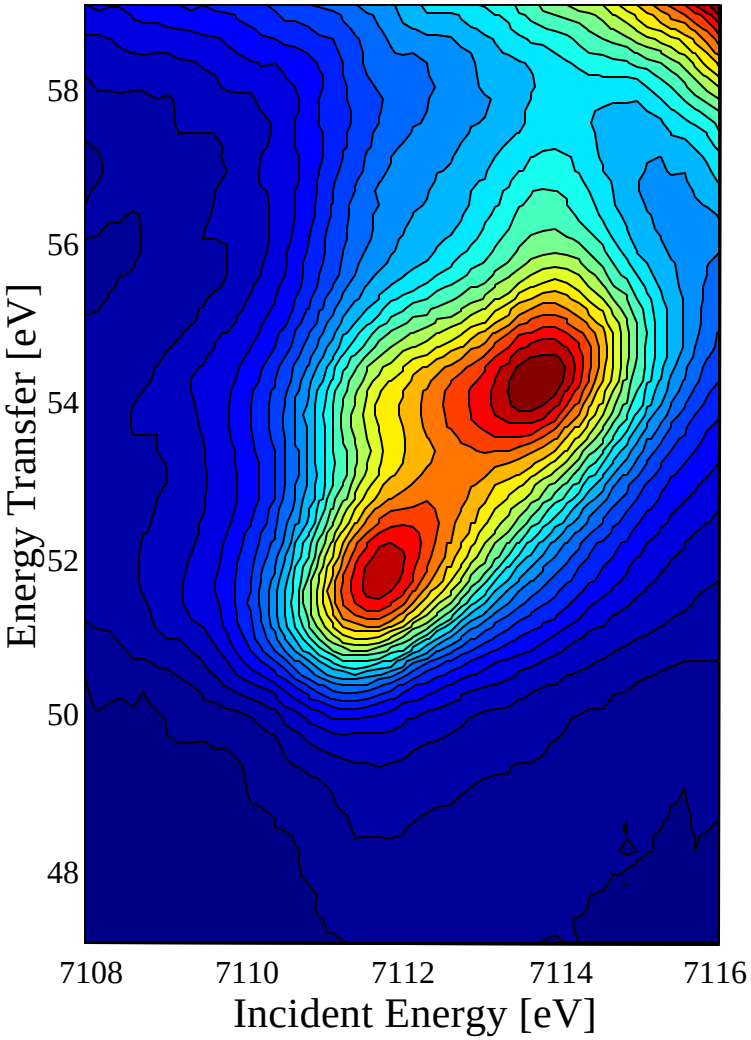


Fe^{2+} in Fayalite (Fe_2SiO_4) O_h

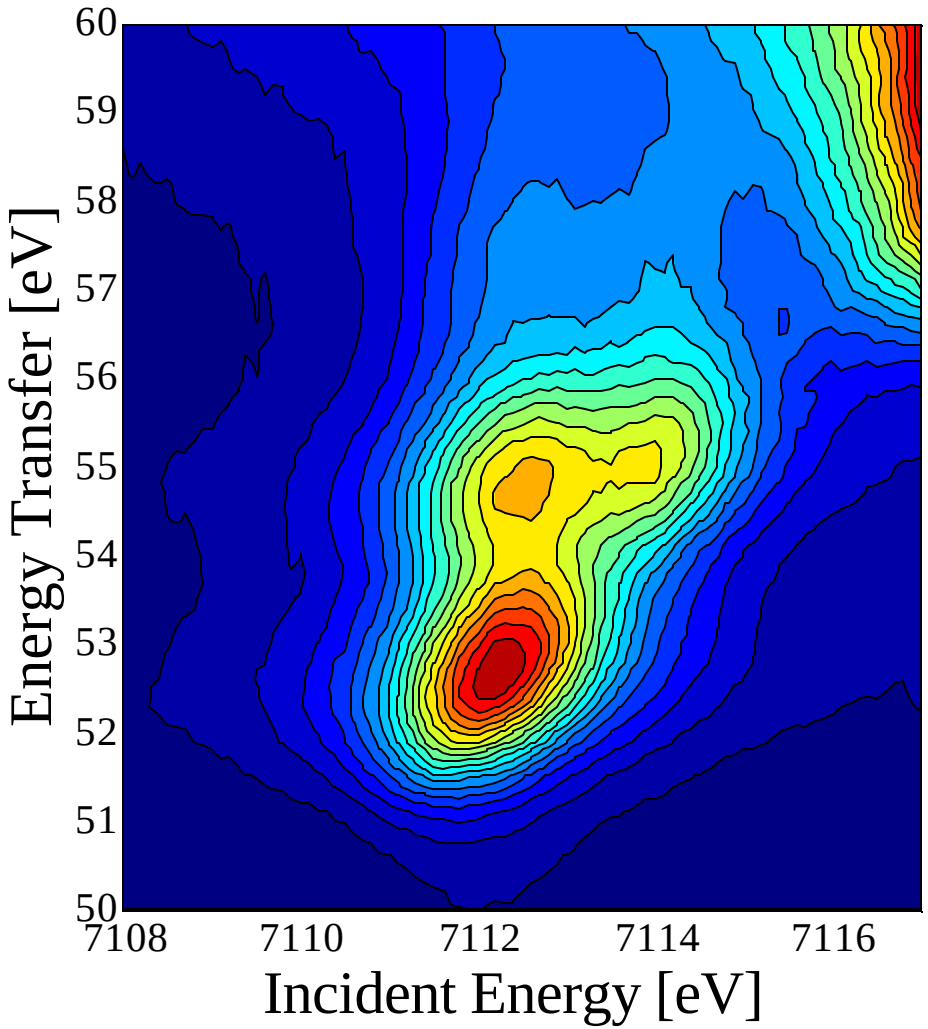


RIXS of Iron compounds

Fe^{2+} in $Fe_{0.05}Mg_{0.95}O$

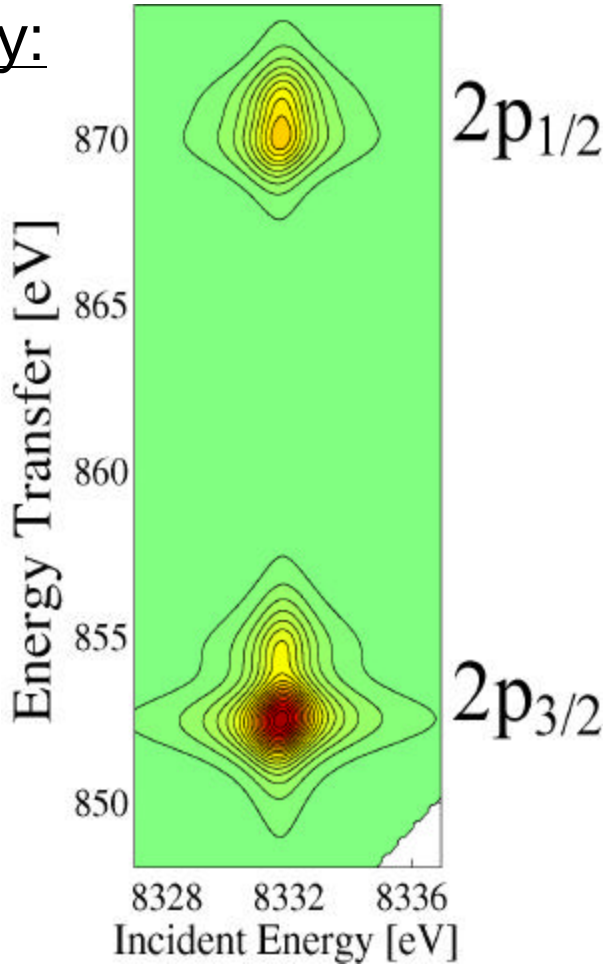


Fe^{2+} in Fayalite (Fe_2SiO_4) O_h



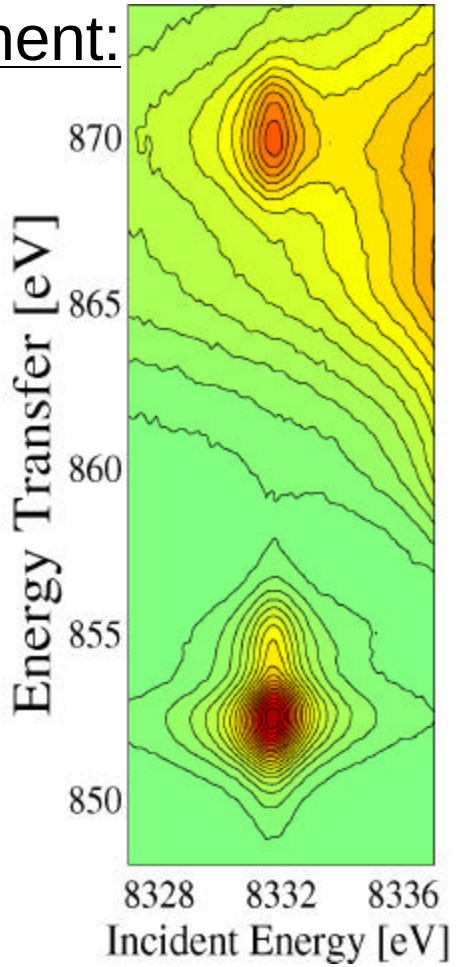
Comparison with Calculations

Theory:

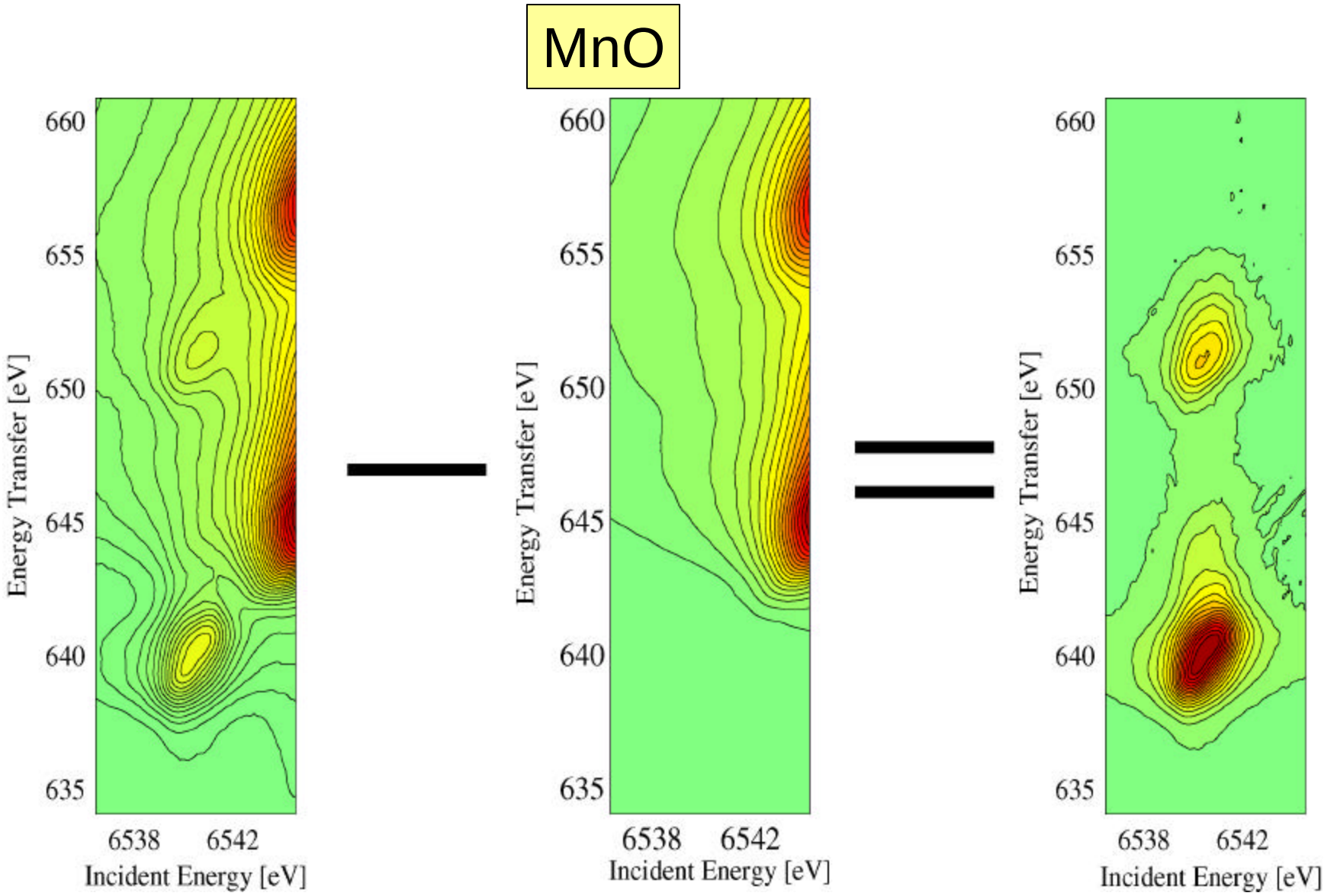


NiF_2

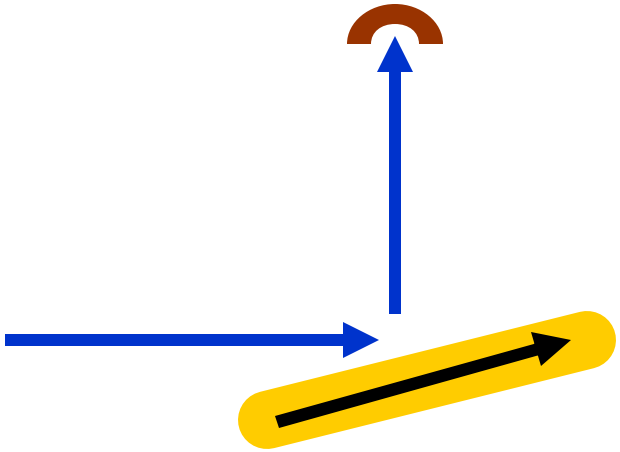
Experiment:

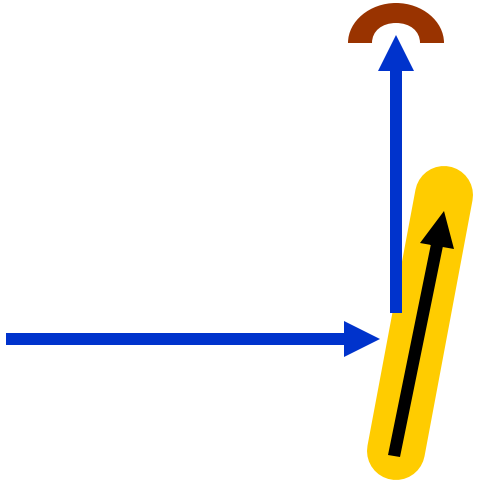


Background Subtraction



Application to Magnetic Materials





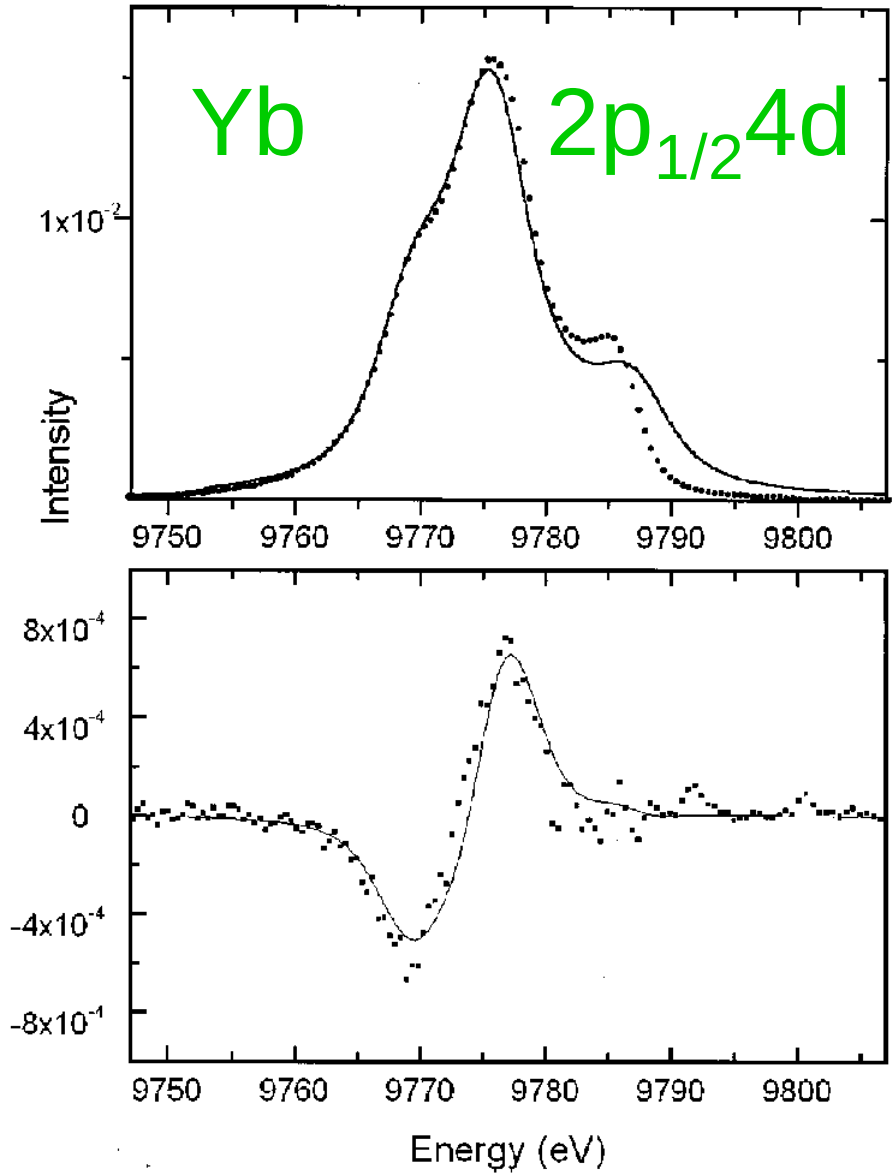
1s edge MCD: small
2p edge MCD: UHV

1s2p RIXS MCD: large

Hard x-rays (in + out)
also large MLD

Phys. Rev. B.
62, 379 (2000)

Application to Magnetic Materials



$Yb_3Fe_5O_{12}$ $4f^{13}$

Hard X-rays

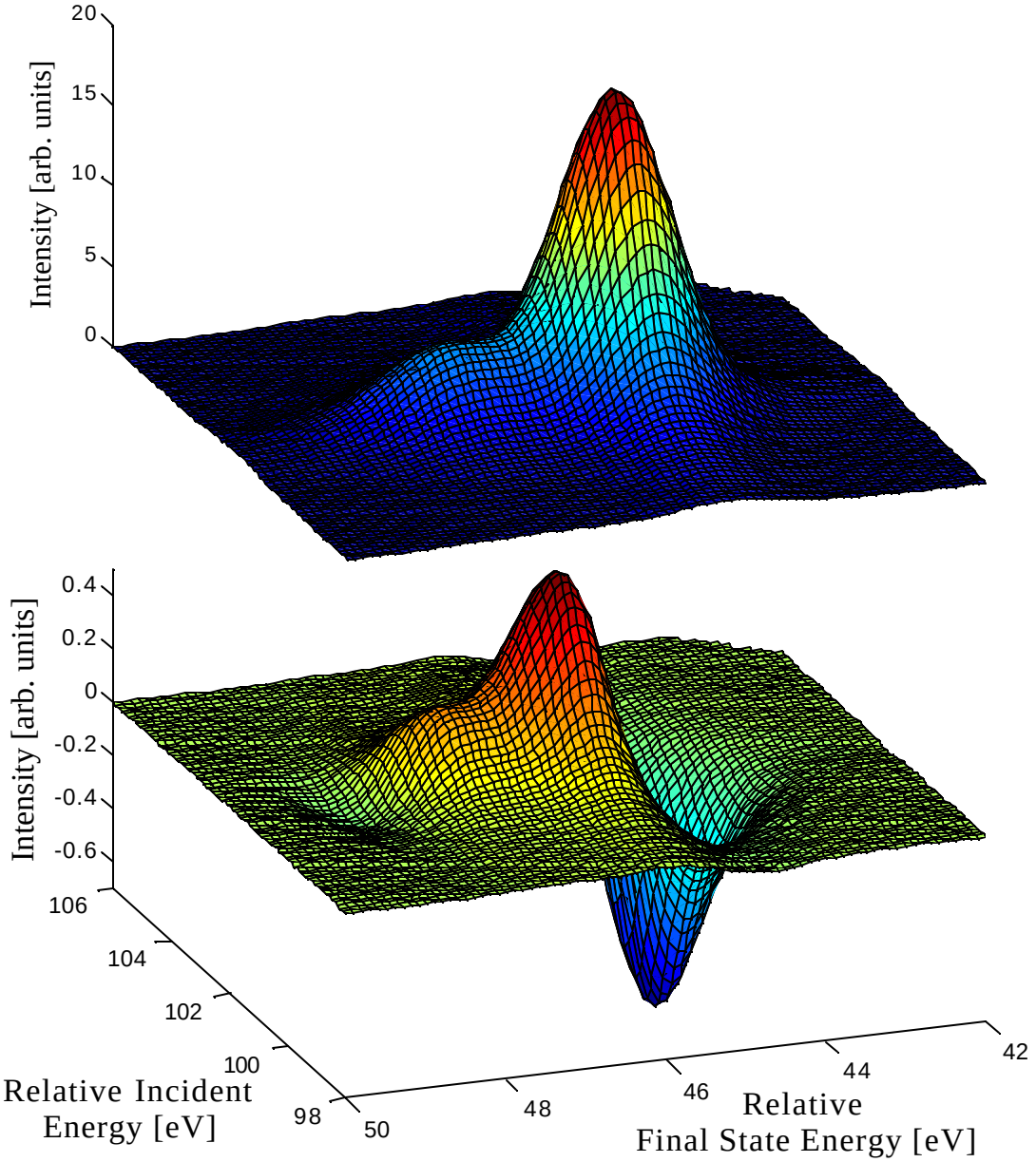
- Buried Layers
- μ(P,T,..)

Phys. Rev. B. 62, 379 (2000)

Application to Magnetic Materials

Ni(II) high-spin
1s2p RIXS

MCD



New possibilities in X-ray Spectroscopy

- Soft x-ray Spectra with Hard X-rays
- Valence Selective XANES and EXAFS
- Spectral Sharpening

Catalysis:

Valence and Symmetry under reaction conditions

Biocatalysis:

Nature of active Mn site

Magnetic Materials:

Magnetic Moment at high pressure