

# Röntgenspektroszkópiák az anyagszerkezet-kutatásban

Bajnóczi Éva és Németh Zoltán  
MTA Wigner FK  
nemeth.z@wigner.mta.hu

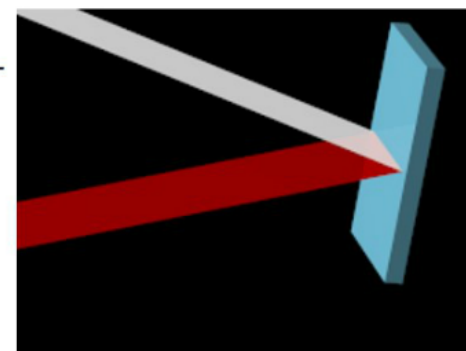
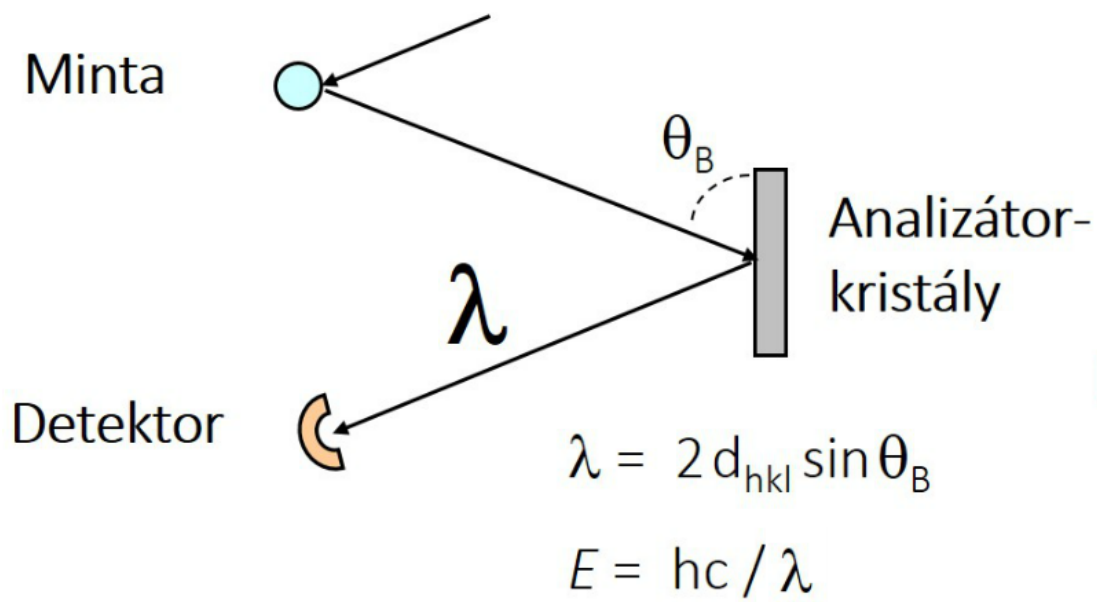
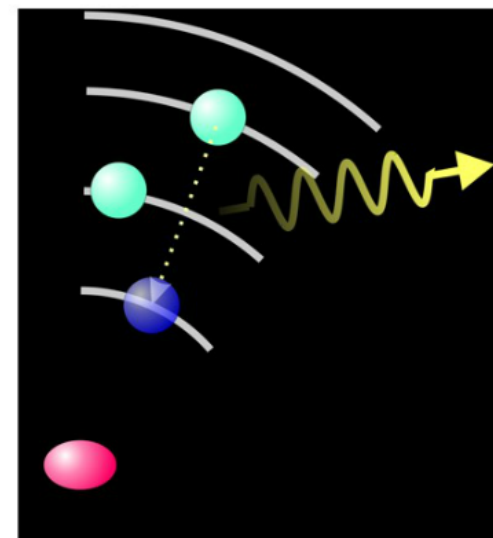
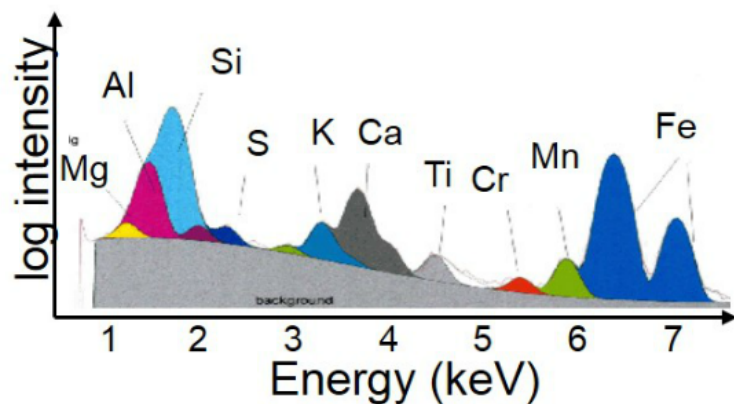
- 1) általános bevezető, módszerek csoportosítása, eszközök
- 2) legfontosabb röntgenabszorpciós technikák
- 3) specifikusabb módszerek: XES, RXES, XMCD

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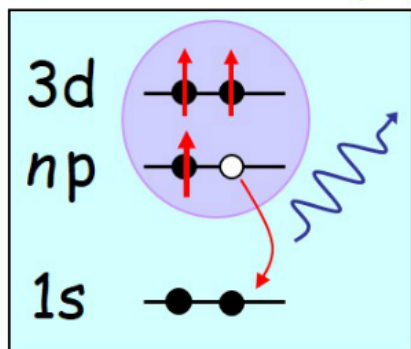
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# X-ray emission spectroscopy (XES)

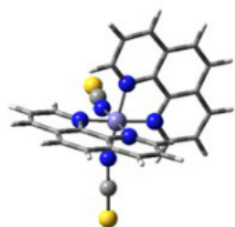


# 1s XES spinállapot-függése

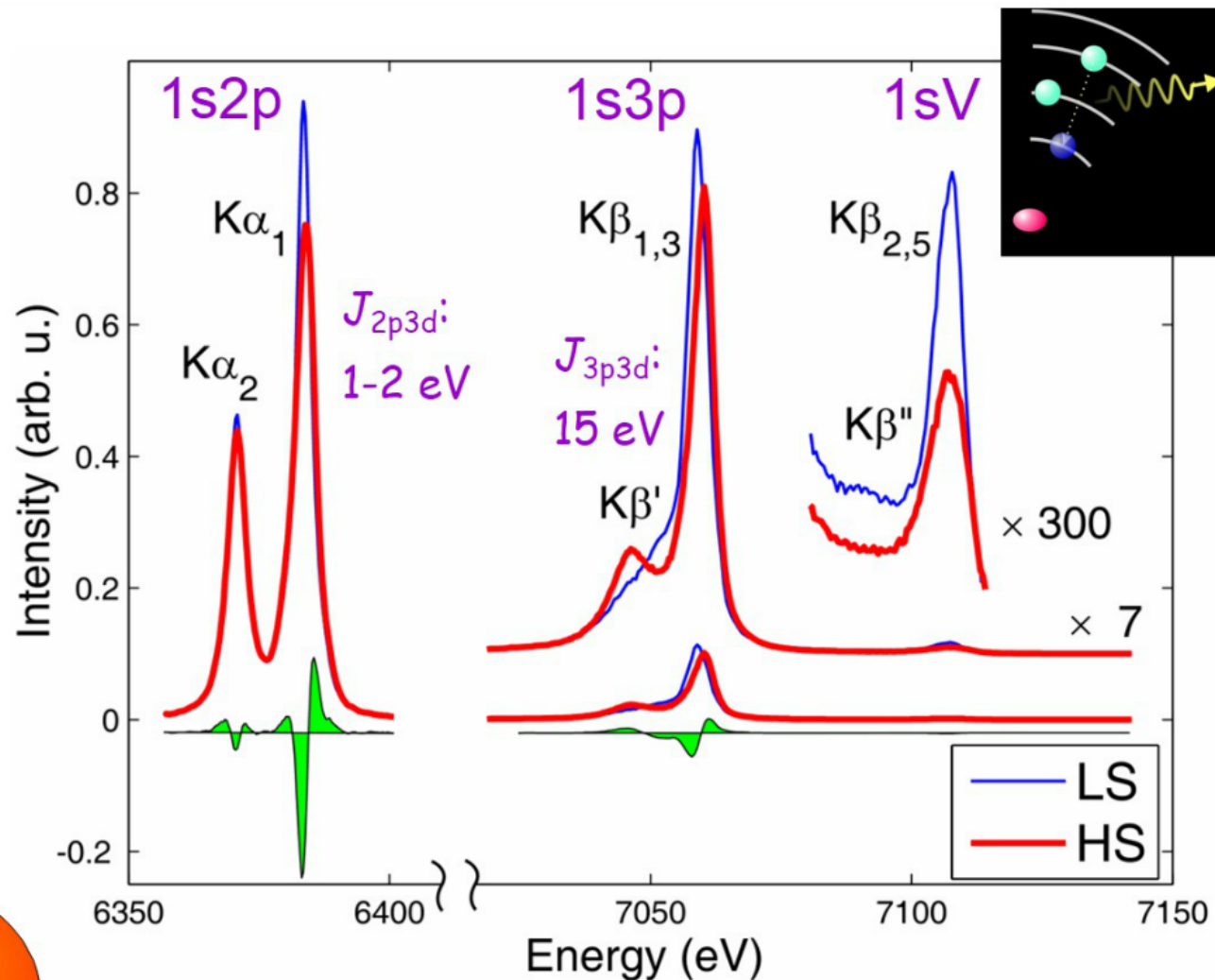
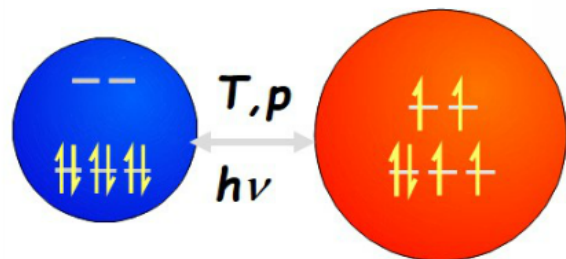
kicszerélődés ( $J$ )



$\text{Fe}^{\text{II}} - 3d^6$

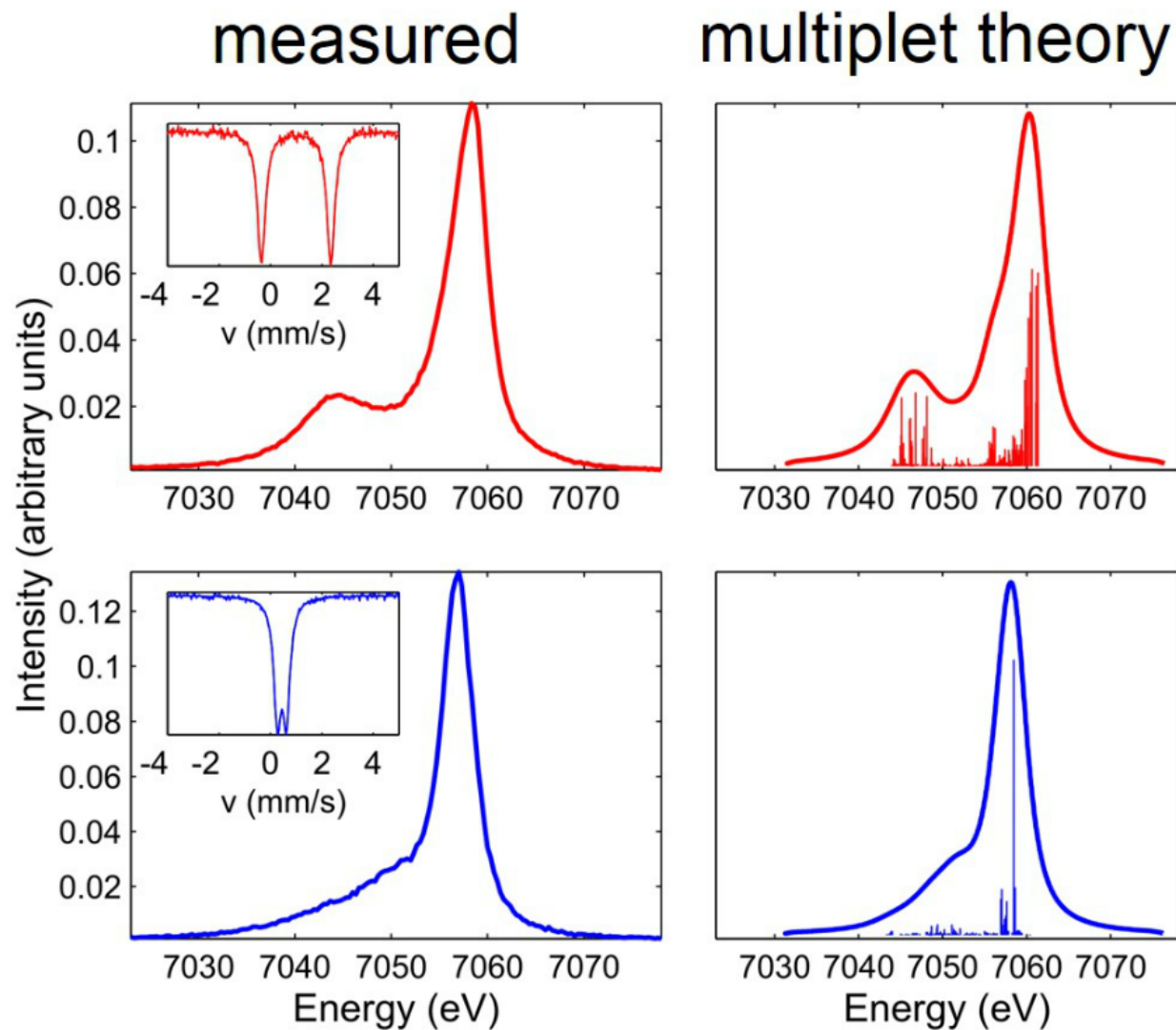
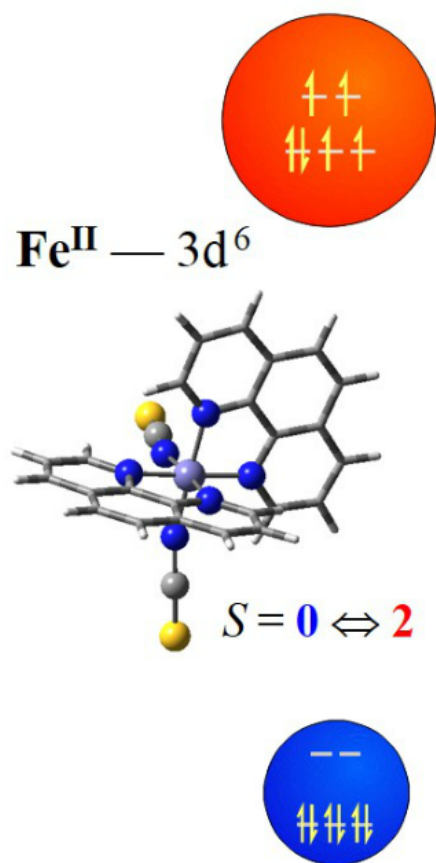


$S = 0 \Leftrightarrow 2$



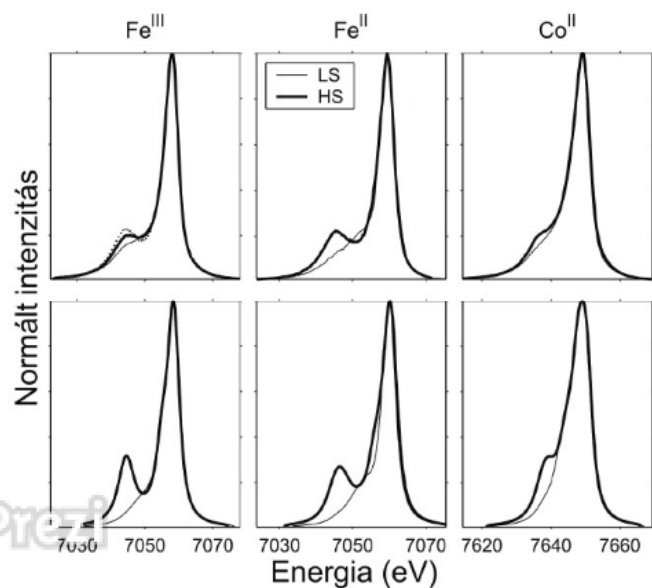
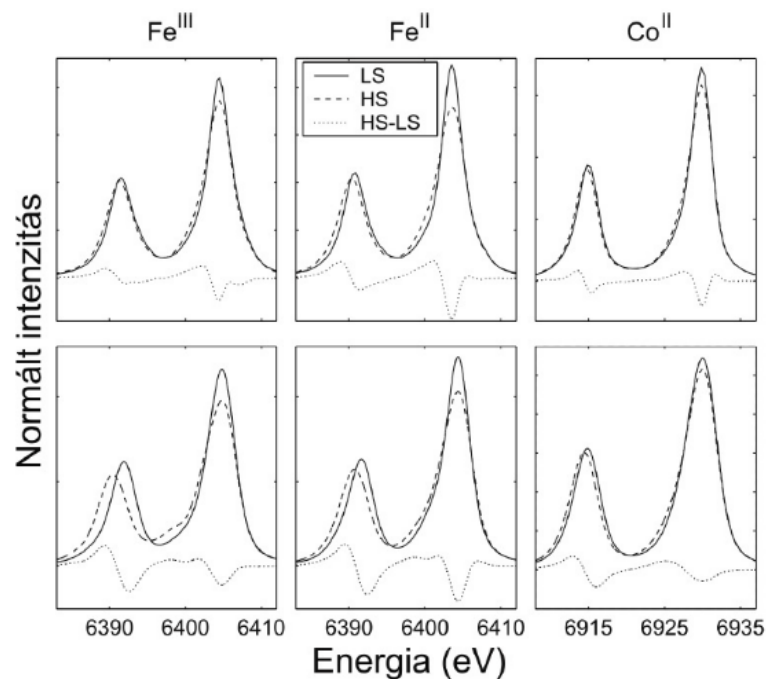
G. Vankó *et al.*, *J. Phys. Chem. B* **110** (2006) 11647

# 1s3p XES spinállapot-függése

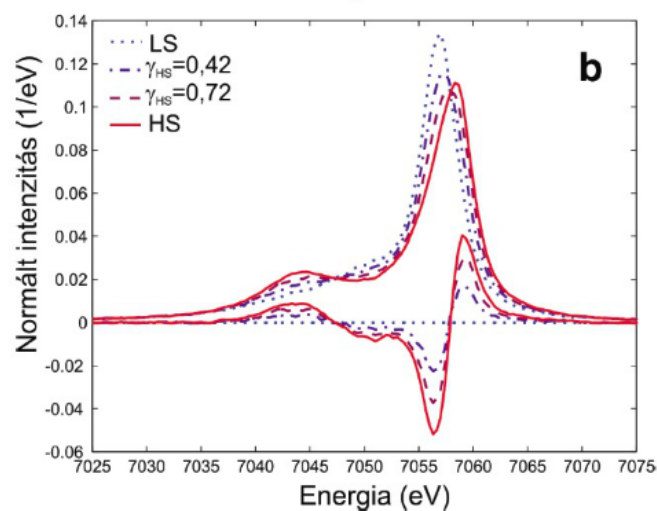
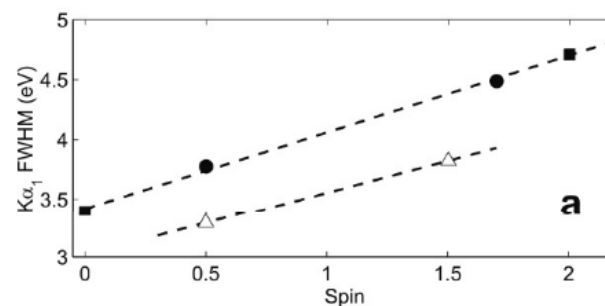


G. Vankó, F. de Groot, *Phys. Rev. B* **75** (2007) 177101.

# spinállapot meghatározása



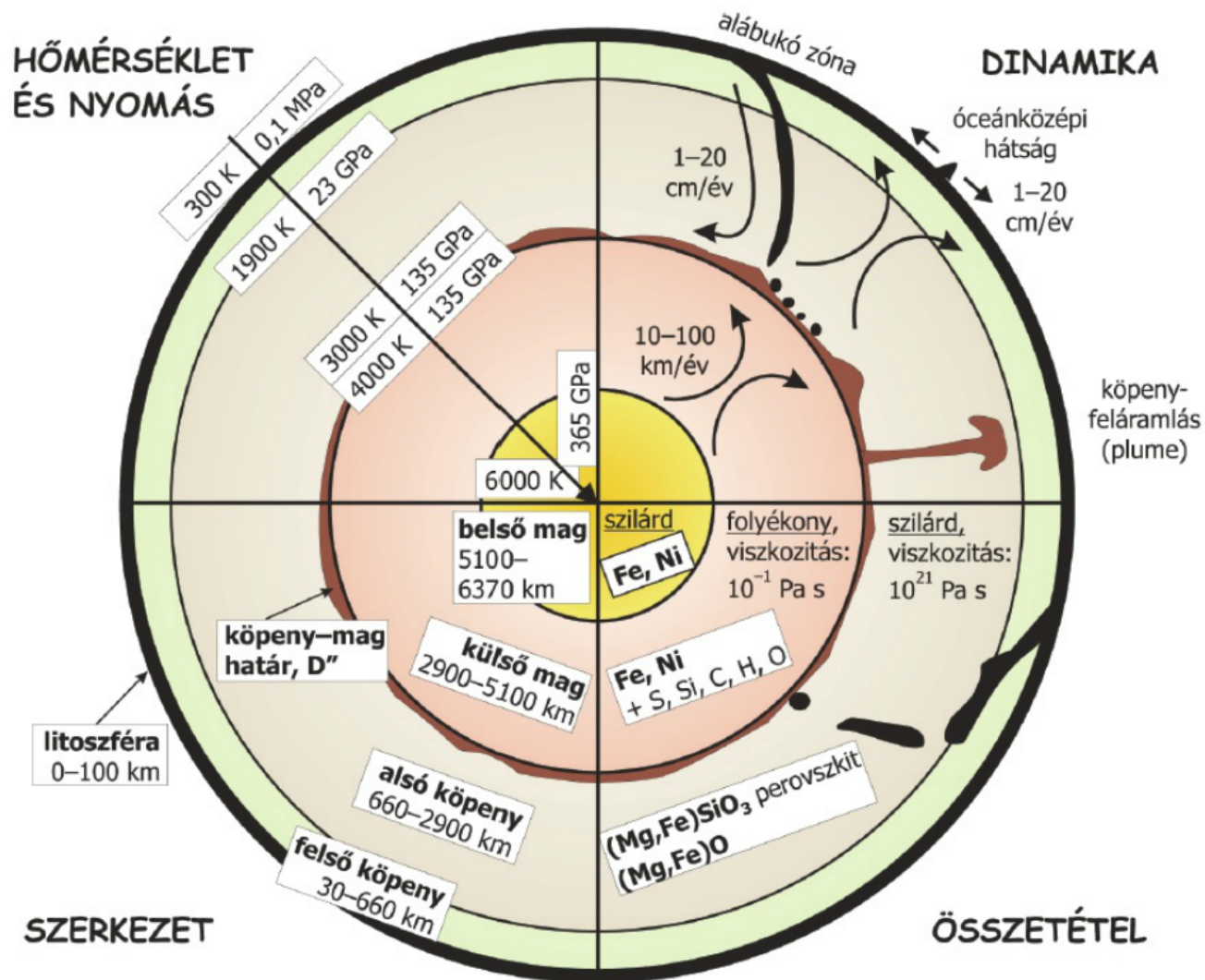
vonalszélességekből



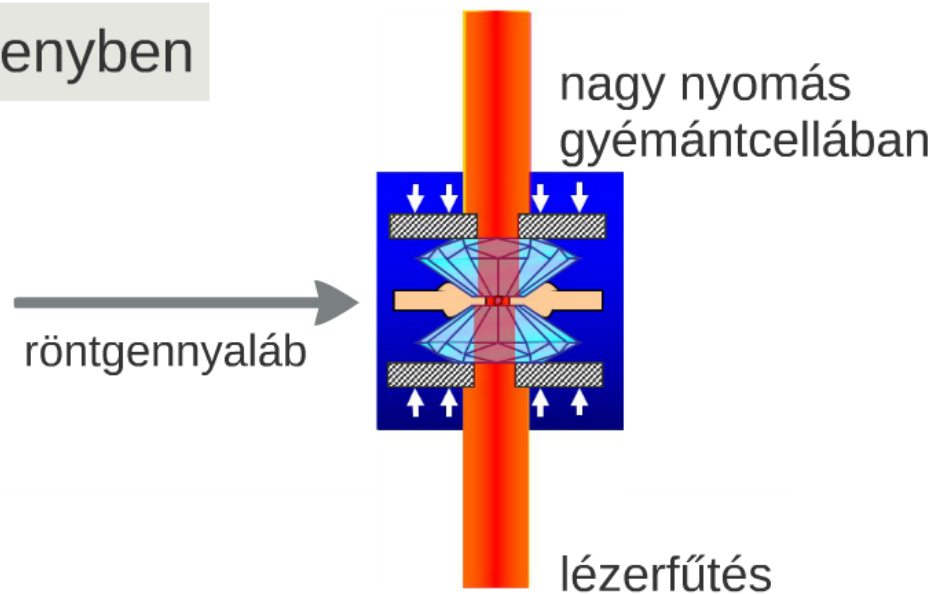
IAD módszer:  
integrált abszolút különbségek



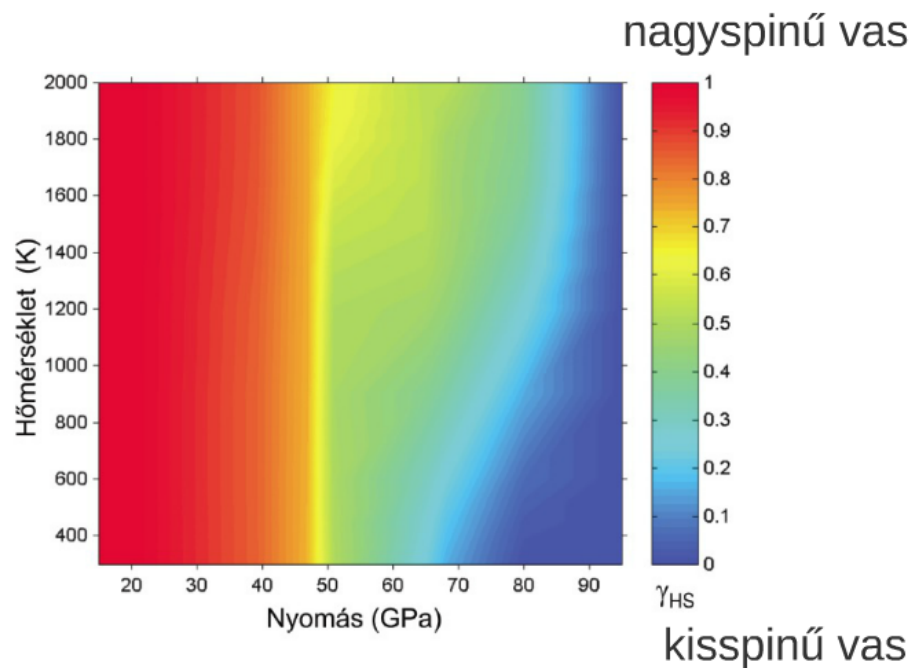
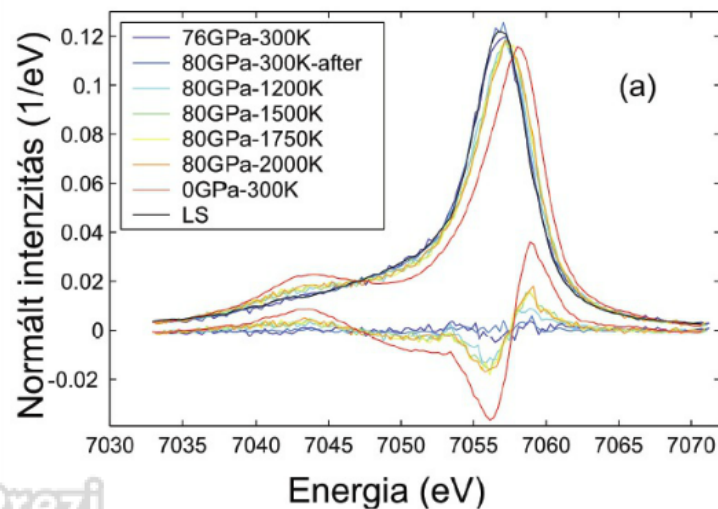
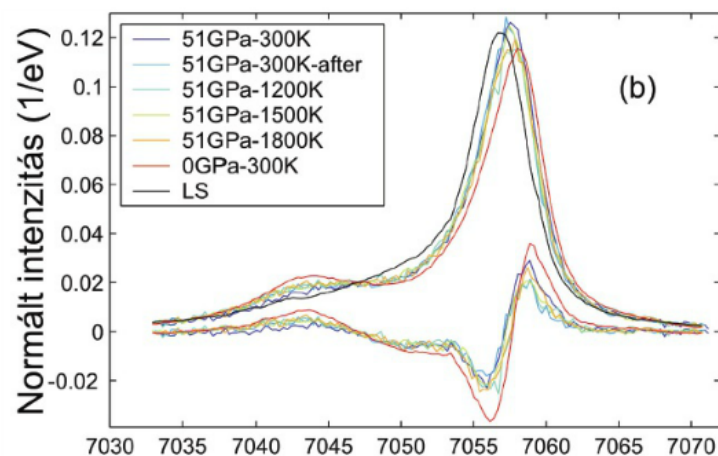
# a Föld szerkezete



# spinállapotváltozás az alsó köpenyben

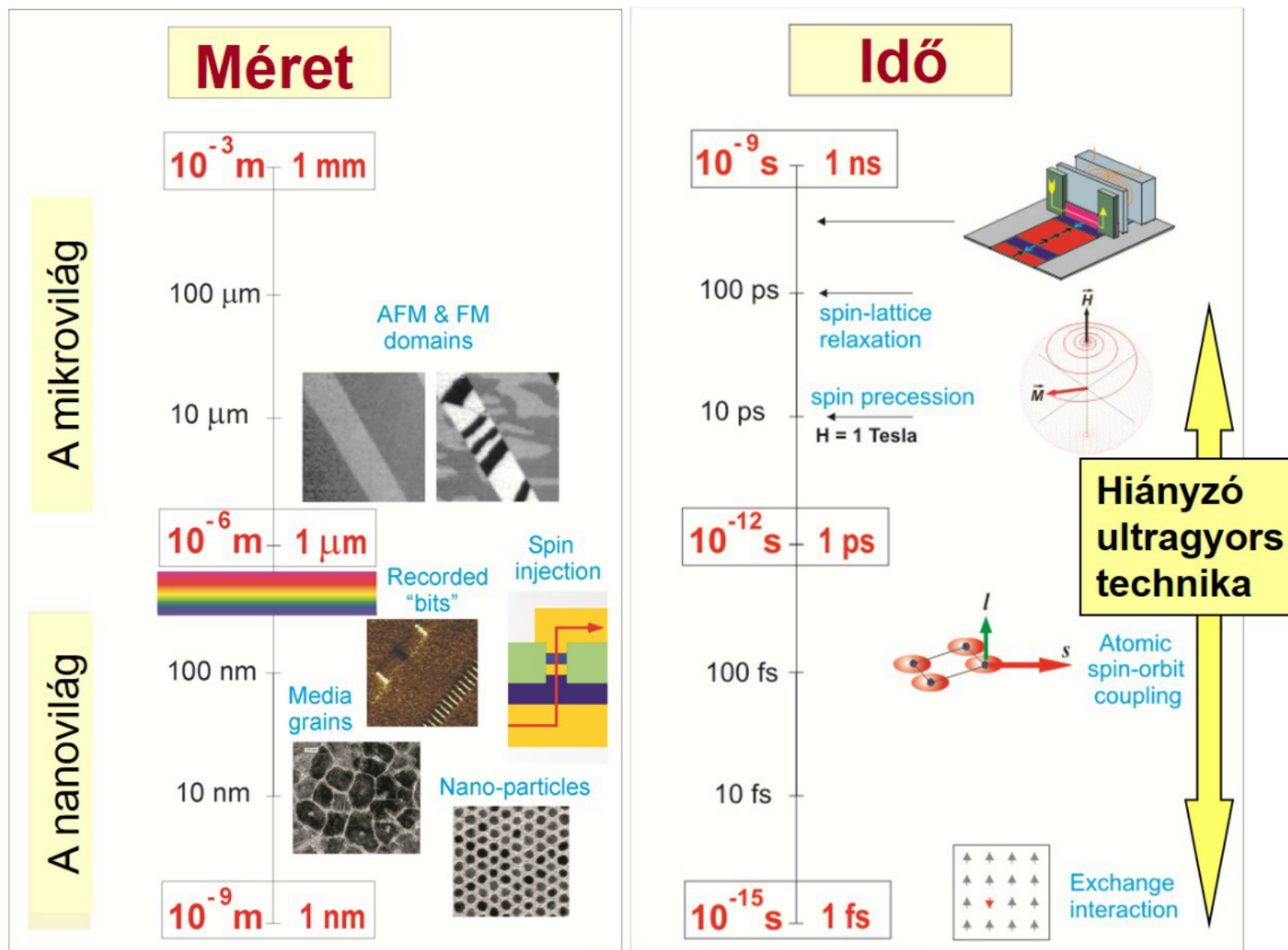


$\text{Mg}_{0.75}\text{Fe}_{0.25}\text{O}$  ferroperiklász

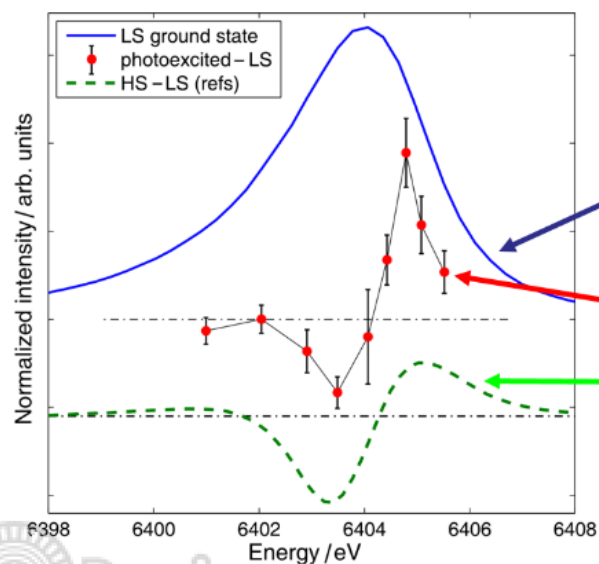
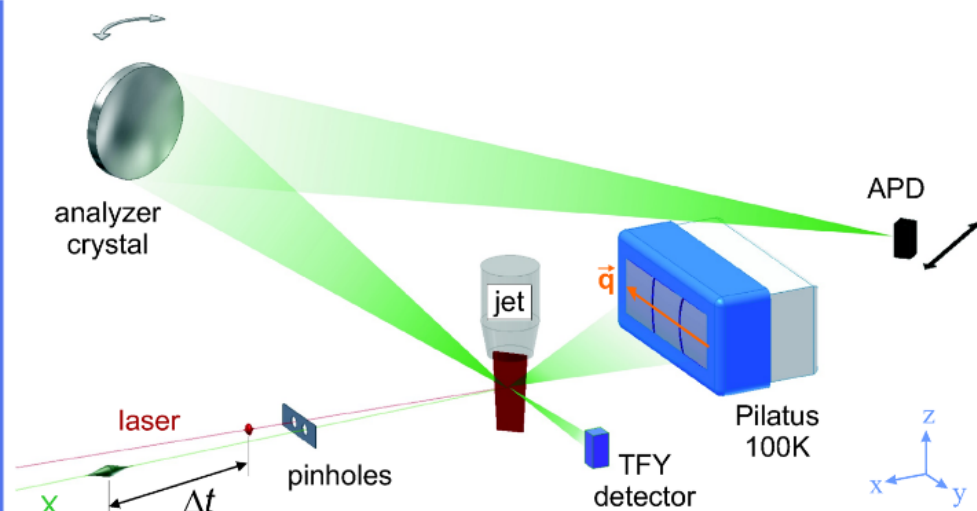
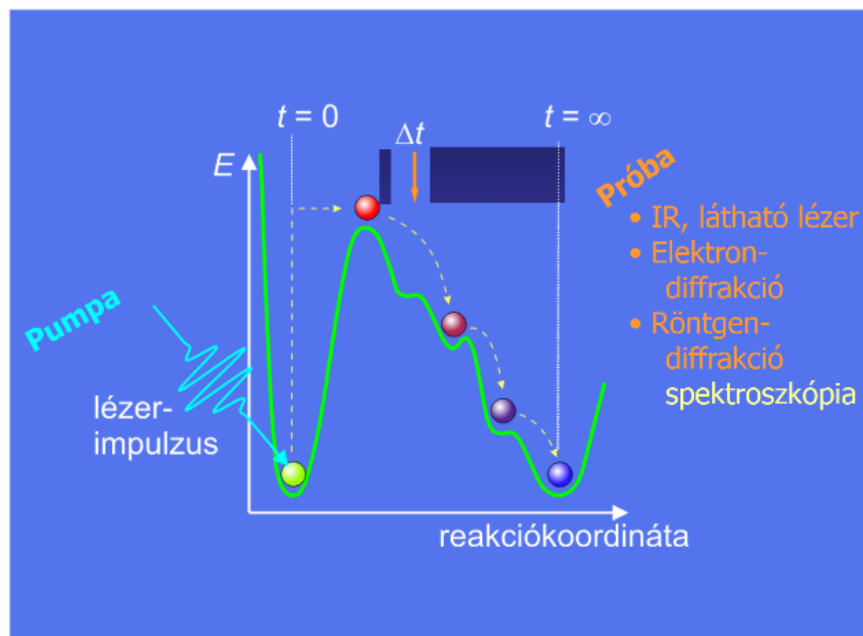




# kapcsolható molekulák



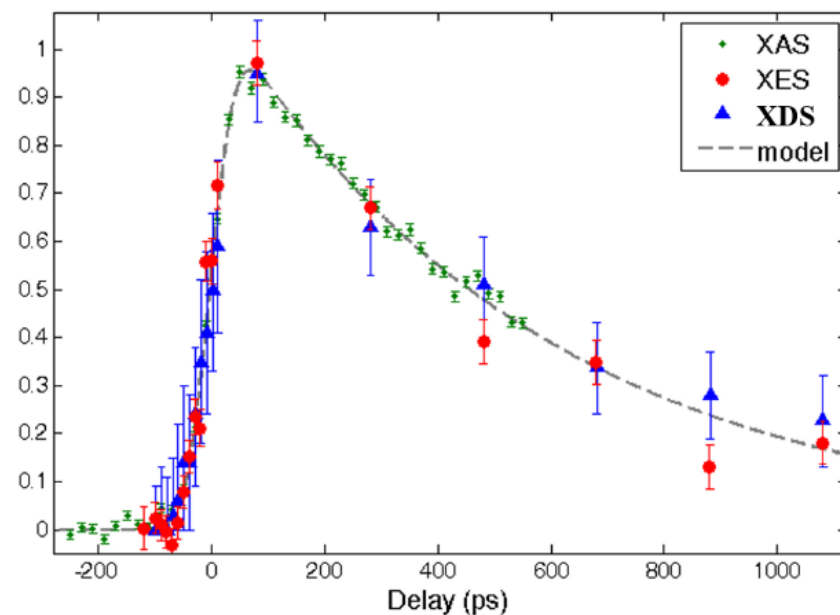
# optikai pumpa - XES szonda mérés szinkrotronnál



LS  $[\text{Fe}(\text{bipy})_3]^{2+}$   
alapállapot

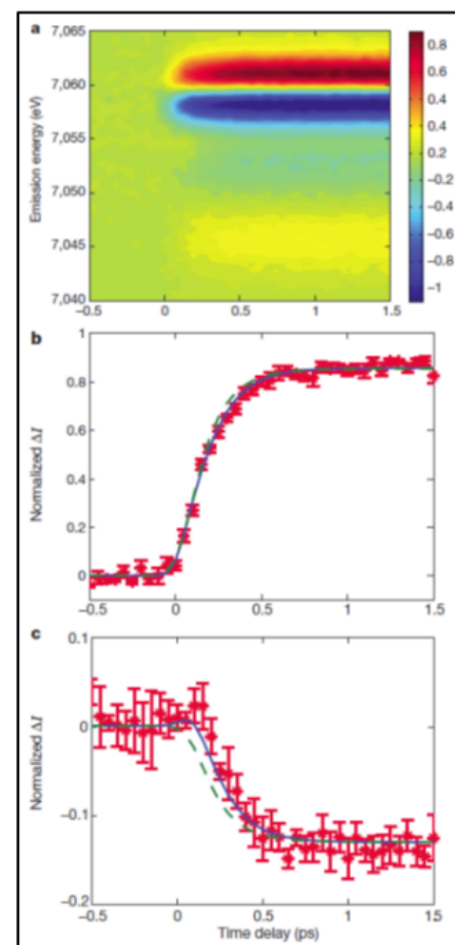
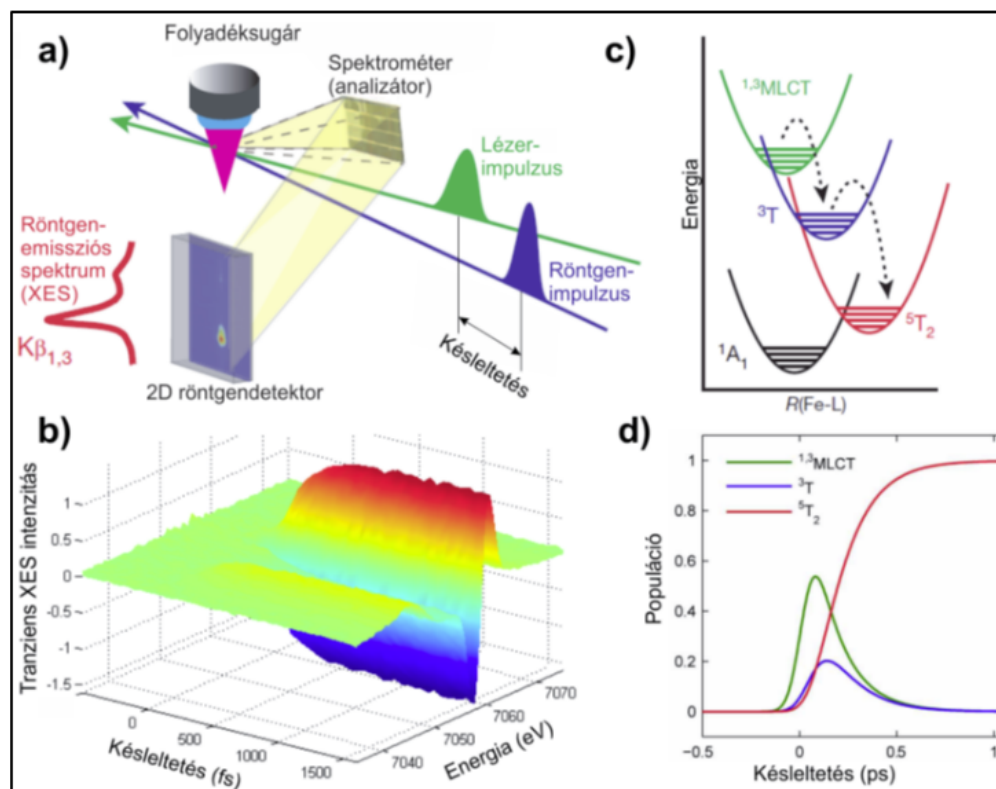
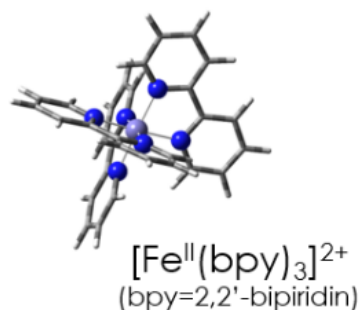
mért adatok

várt spektrum  
(10% HS)



J. Phys. Chem. A 2012, 116, 9878

# optikai pumpa - XES szonda mérés XFEL-nél



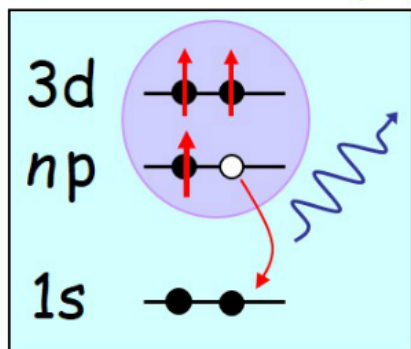
XES különbségi spektrumok az idő függvényében

spektrum-intenzitás különbsége 7061 eV-nál

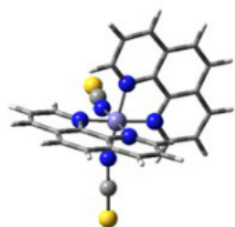
spektrum-intenzitás különbsége 7054 eV-nál

# 1s XES spinállapot-függése

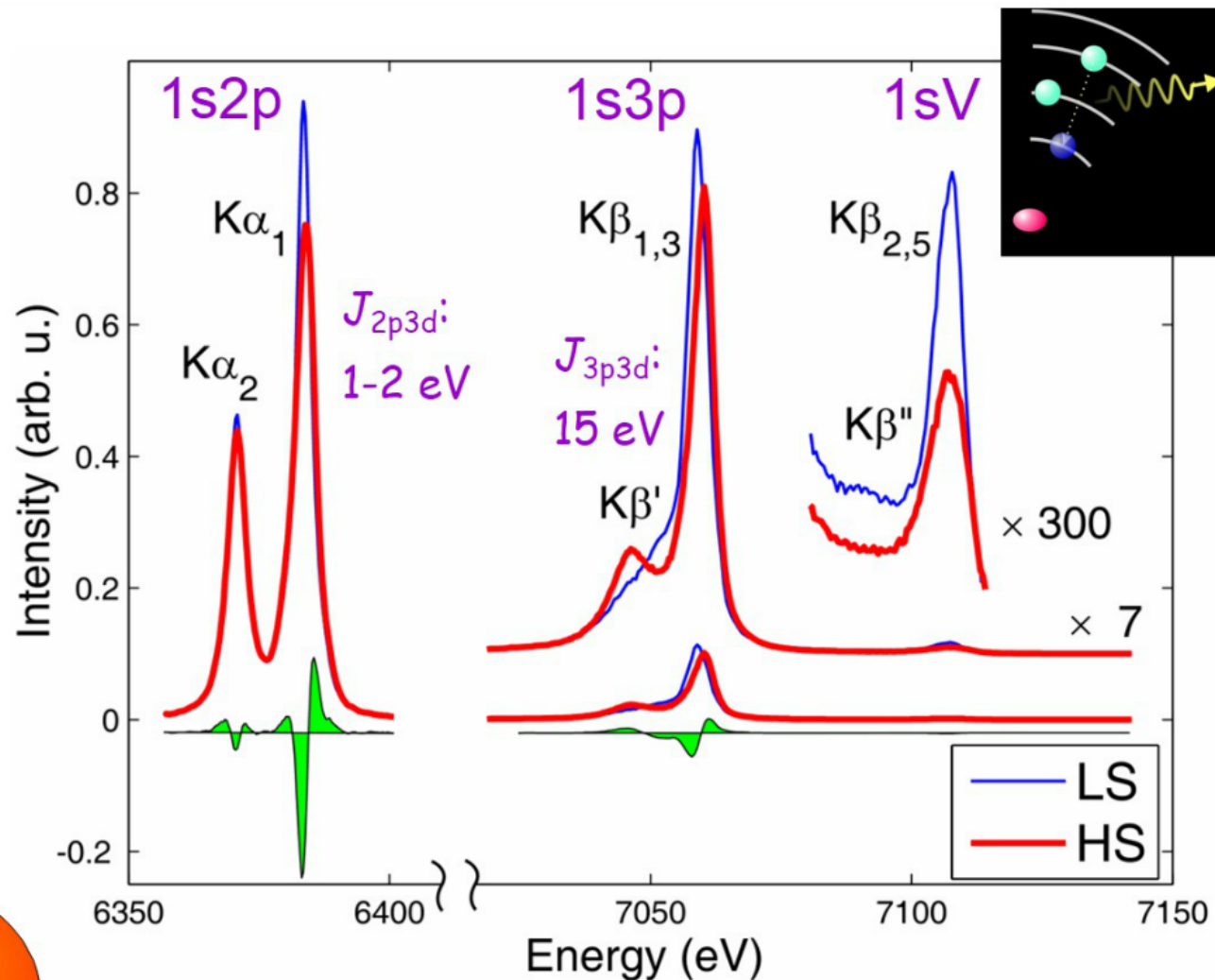
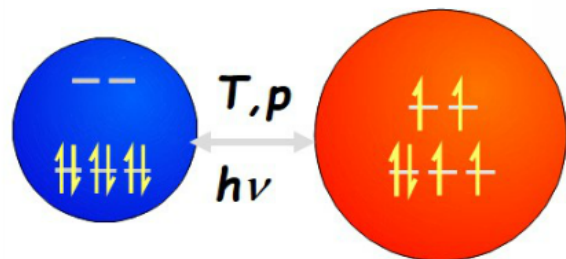
kicszerélődés ( $J$ )



$\text{Fe}^{\text{II}} - 3d^6$

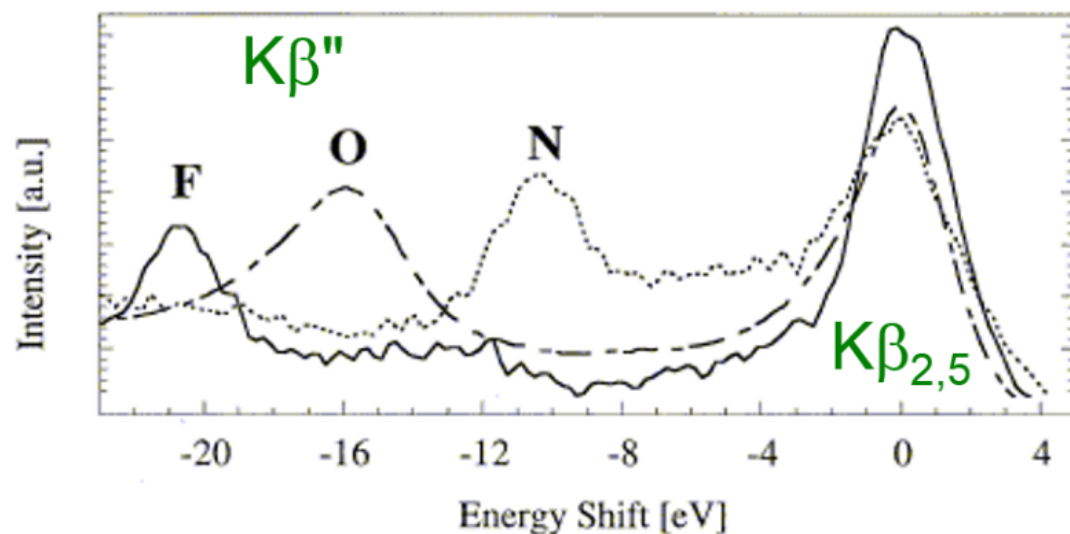


$S = 0 \Leftrightarrow 2$



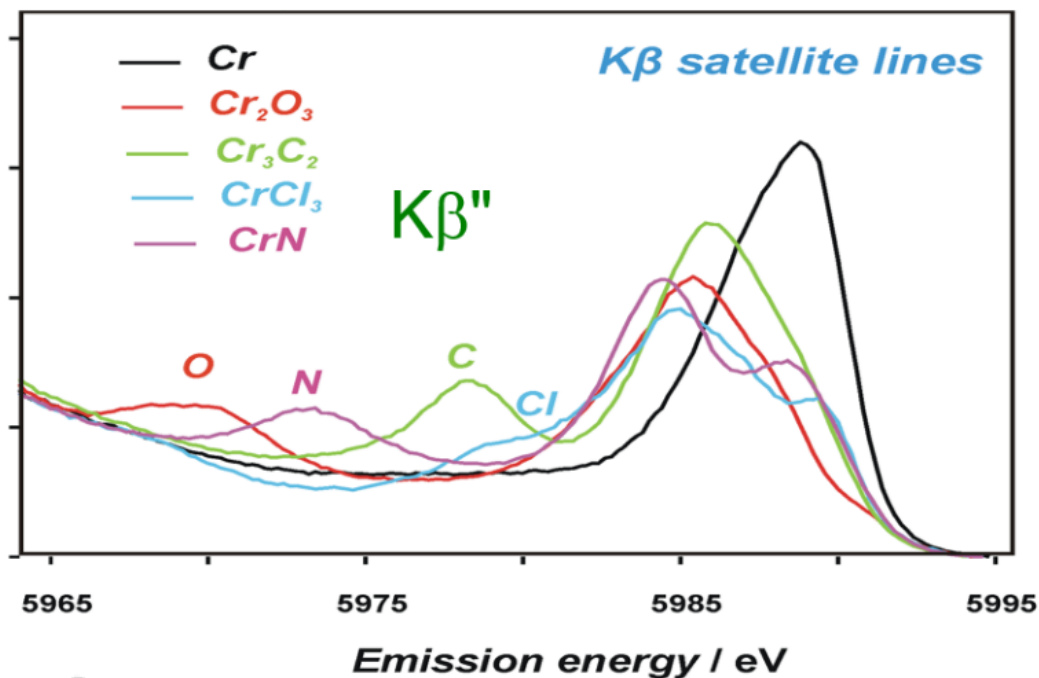
G. Vankó *et al.*, *J. Phys. Chem. B* **110** (2006) 11647

## vegyértékemissziós (aka vtc, valance-to-core) XES



Mn—L

U. Bergmann *et al.*,  
Chem. Phys. Lett.  
302 (1999) 119.

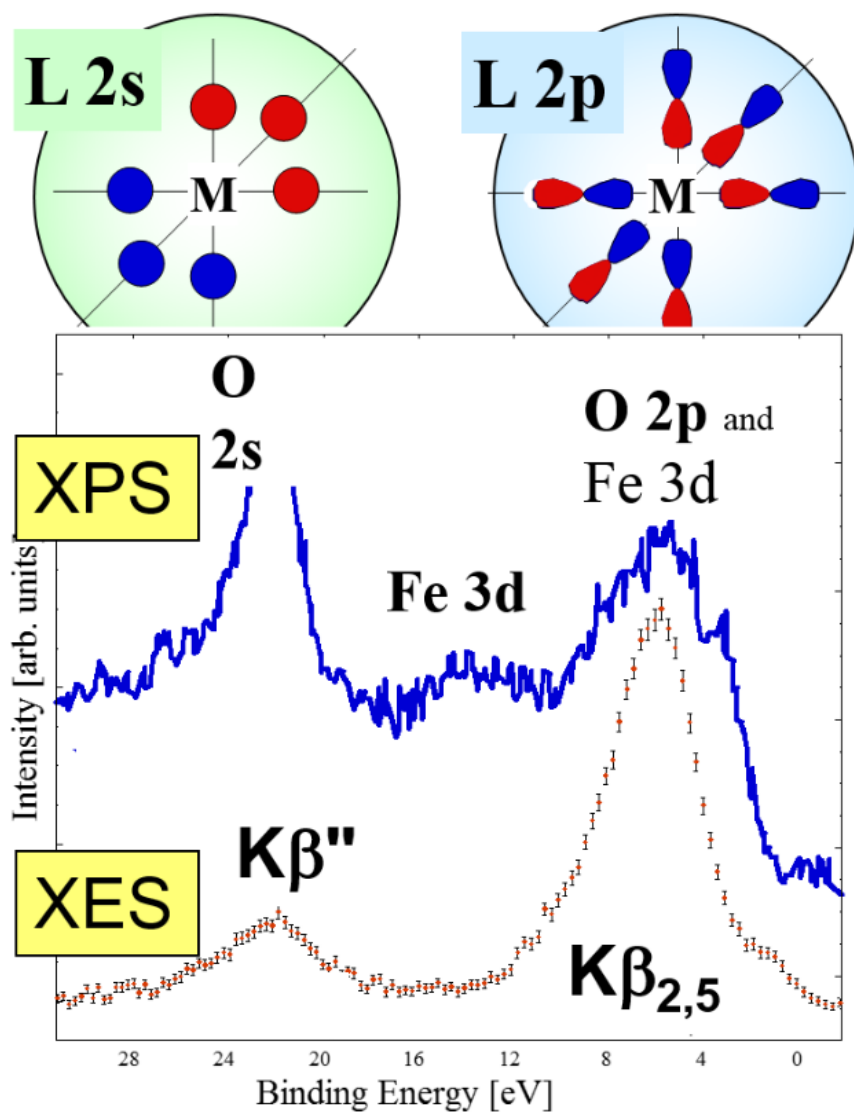


Cr—L

V. A. Safonov *et al.*,  
J. Phys. Chem. B  
110 23192 (2006)



# vtc XES vs. XPS



vegyérték XPS:

O 2s, 2p, Fe 3d

vegyérték-XES:

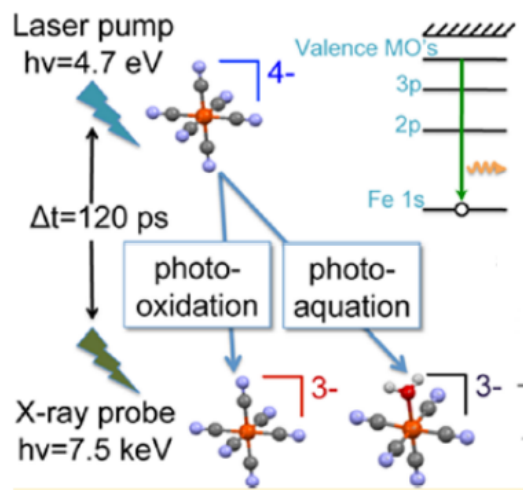
O 2s, O 2p

- azonos végállapotok
- XES-nél dipólus kiválasztási szabályok
- XES tömbi információt ad

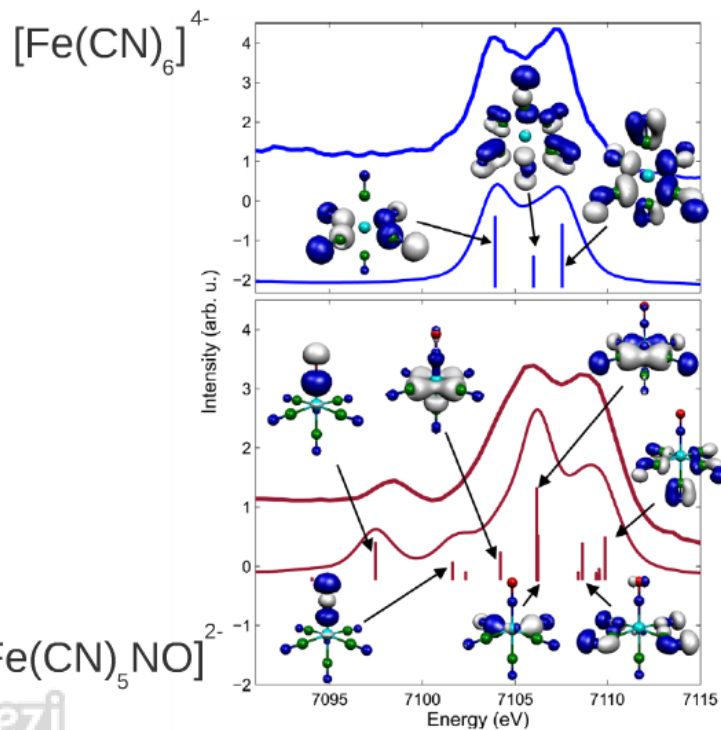
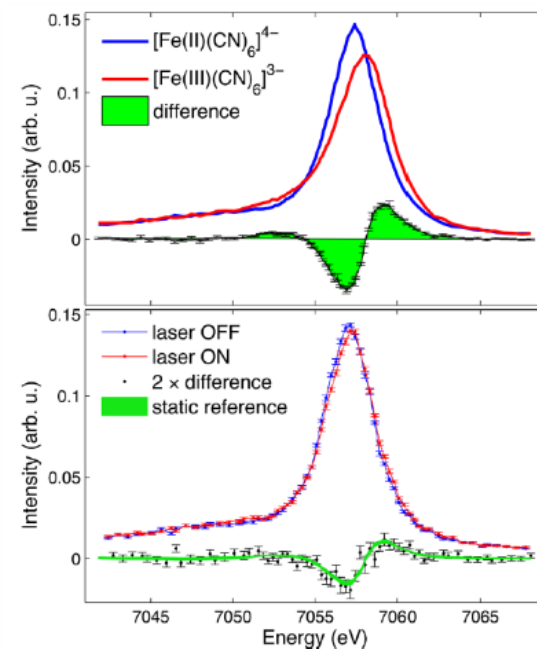




# vtc XES pumpa-szonda kísérletben

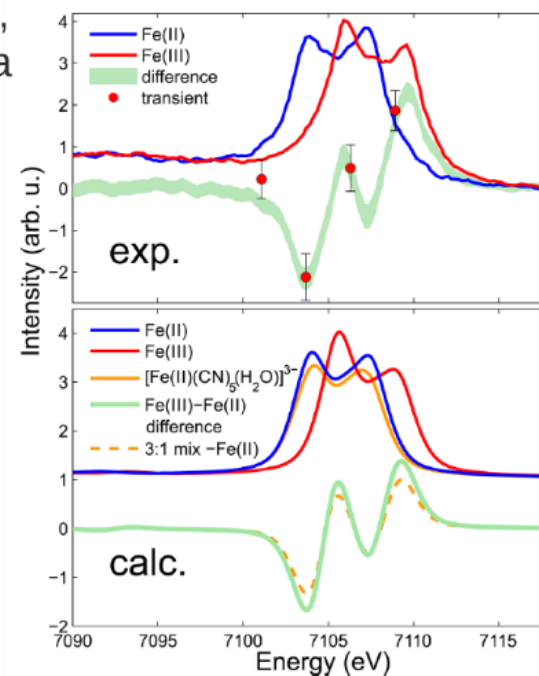


$K_{\beta}$  spektrumok:

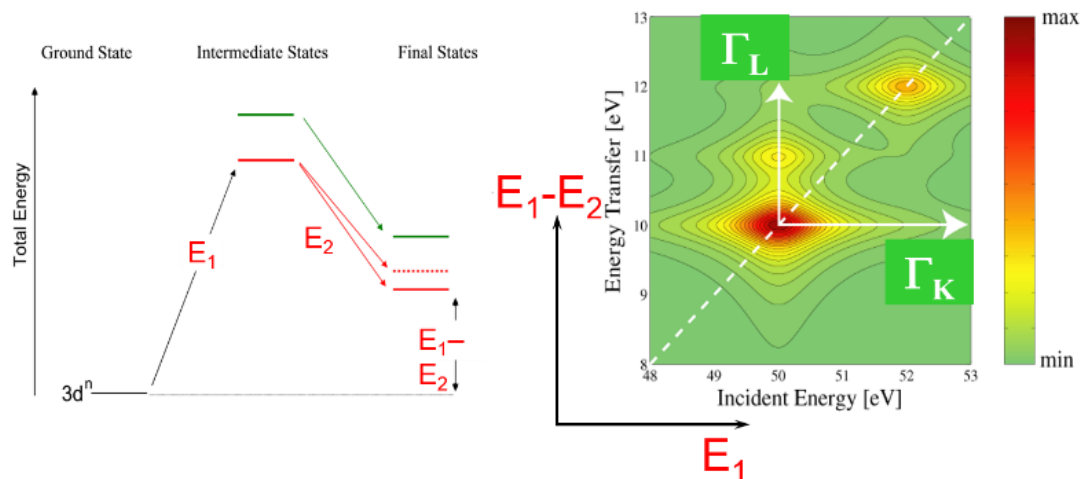


2012, APS (USA),  
Johann-geometria

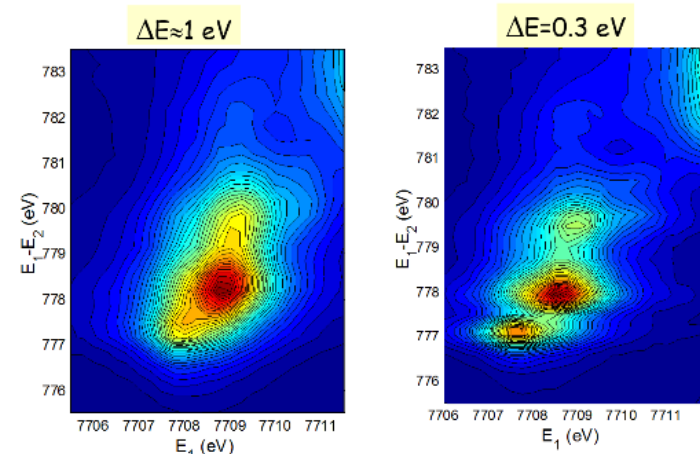
vtc-XES:  
4 pont / éjszaka



# rezonáns röntgenemissziós spektroszkópia (RXES)

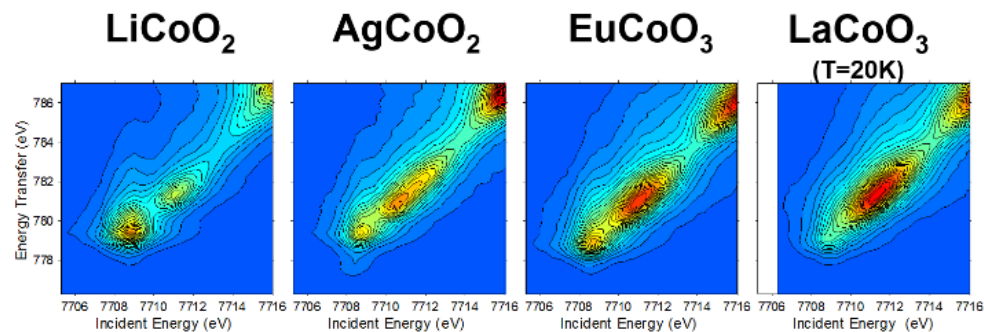
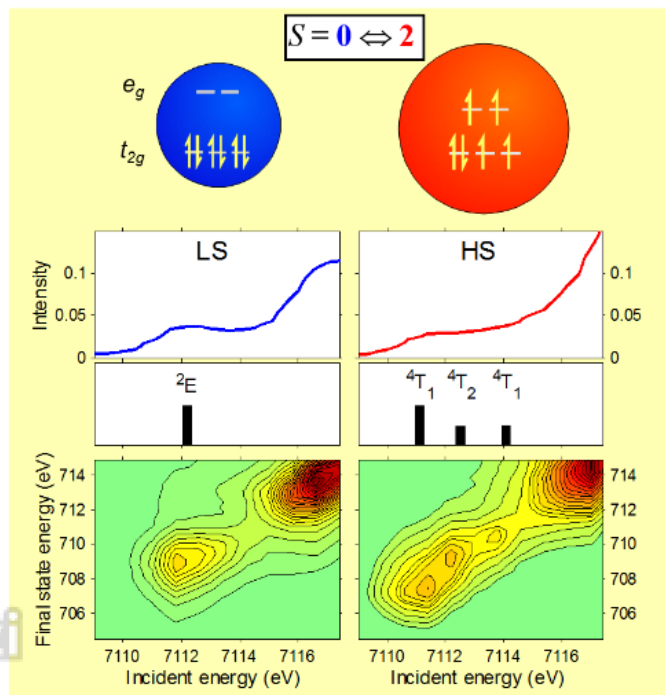


P. Glatzel & U. Bergmann,  
*Coord. Chem. Rev.* **249** (2005) 65.



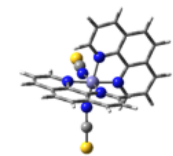
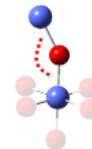
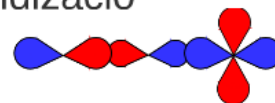
Analyzer: Si(531)  $R = 1$  m  
Mono: Si(440)

Si(531)  $R = 2$  m  
Si(440)

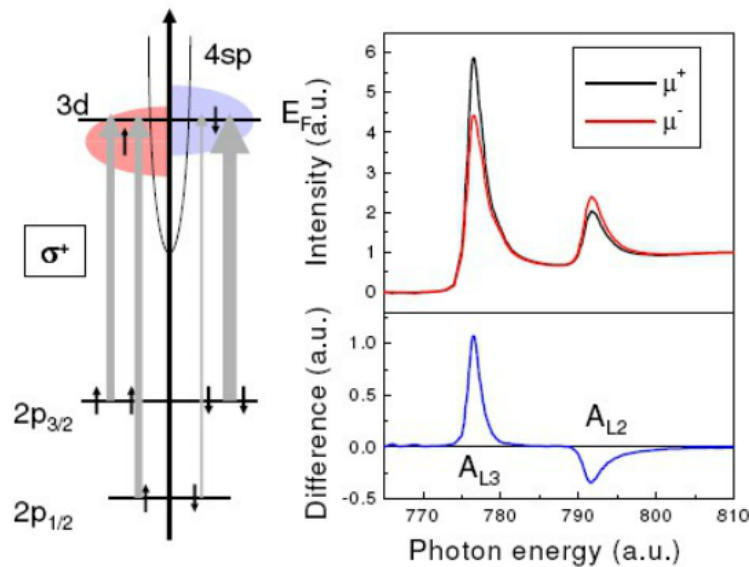


$\angle_{\text{Co-O-Co}}$   $94^\circ$   $97^\circ$   $153^\circ$   $163^\circ$

Co(4p)-O(2p)-Co(3d) hibridizáció  
nő a kötősszöggel



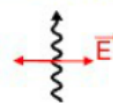
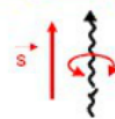
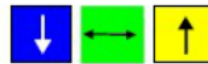
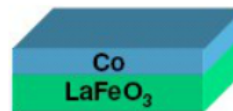
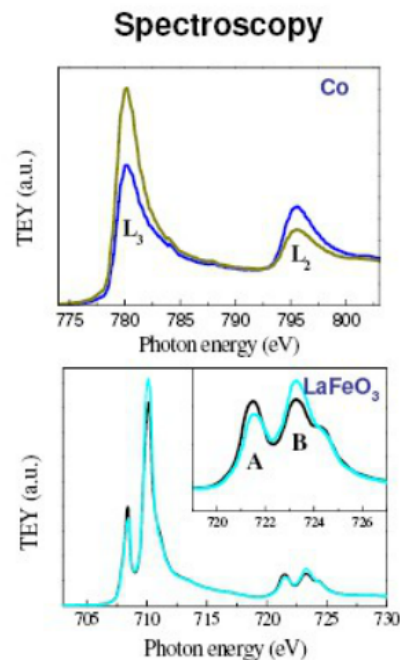
# lágyröntgen mágneses cirkuláris dikroizmus (XMCD)



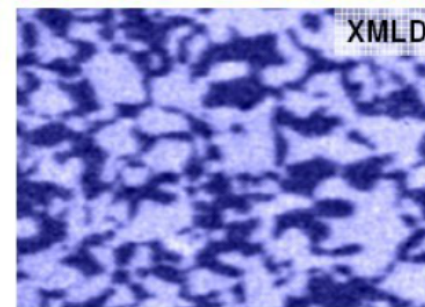
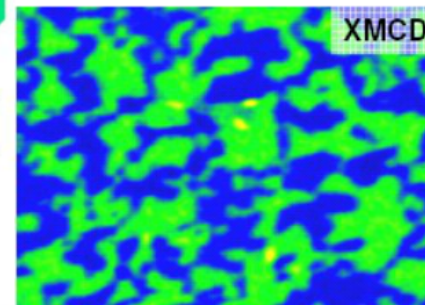
## Sum rules

$$m_s/\mu_B \sim \frac{A_{L3} - 2A_{L2}}{A_{ISO}}$$

$$m_l/\mu_B \sim \frac{A_{L3} + A_{L2}}{A_{ISO}}$$



## Microscopy



# 1s2p RXES - MCD

