Polarization-dependent Resonance Surface X-ray Scattering

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U.S. DEPARTMENT OF ENERGY | Office of Science | Basic Energy Sciences

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Surface Scattering: Anti-Bragg

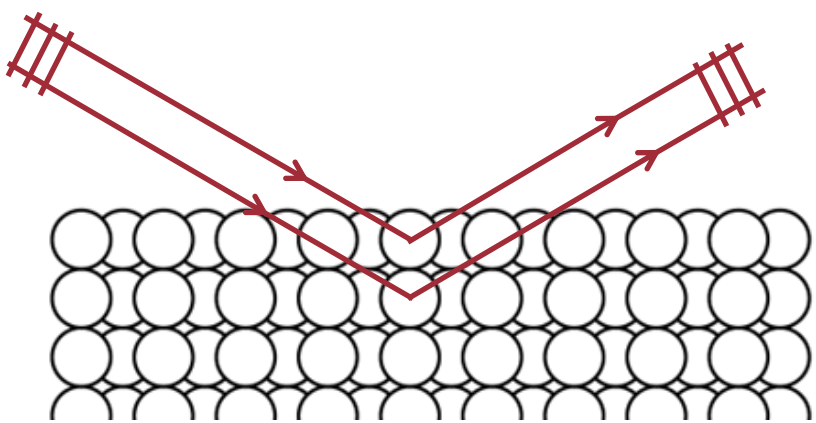
$$S(L,E) = f_{Pt}(L,E) + f_{Pt}(L,E)e^{-i2\pi L} + f_{Pt}(L,E)e^{-2i2\pi L} + \cdots$$

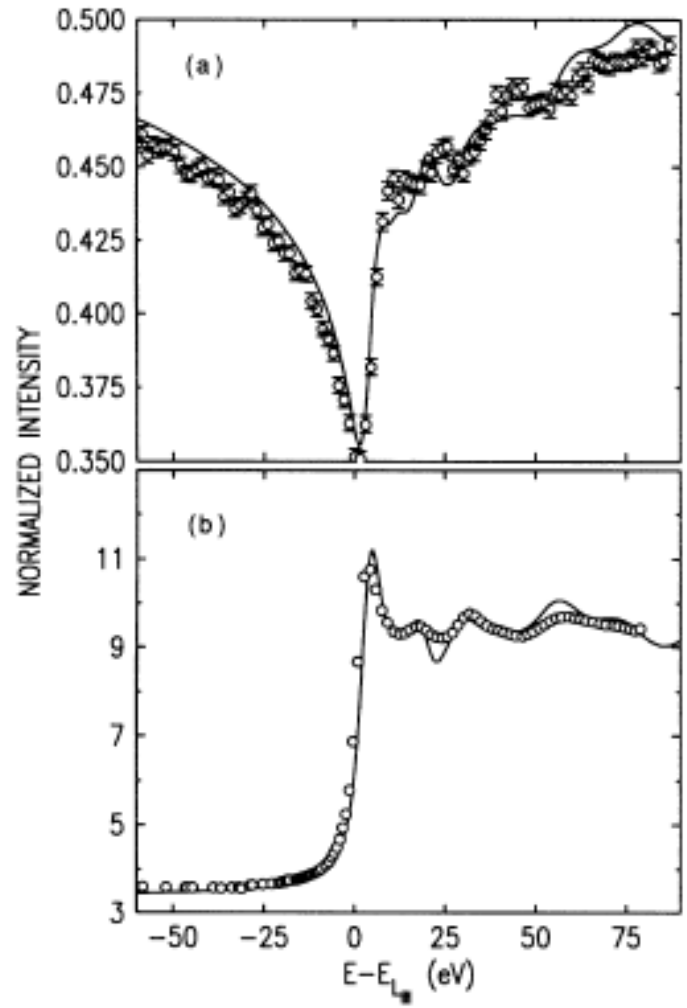
$$= f_{Pt}\left(1 + e^{-i2\pi L} + e^{-2i2\pi L} + \cdots\right)$$

$$= f_{Pt}\sum_{n} e^{-ni2\pi L}$$

$$= \frac{f_{Pt}}{1 + e^{-ni2\pi L}}$$

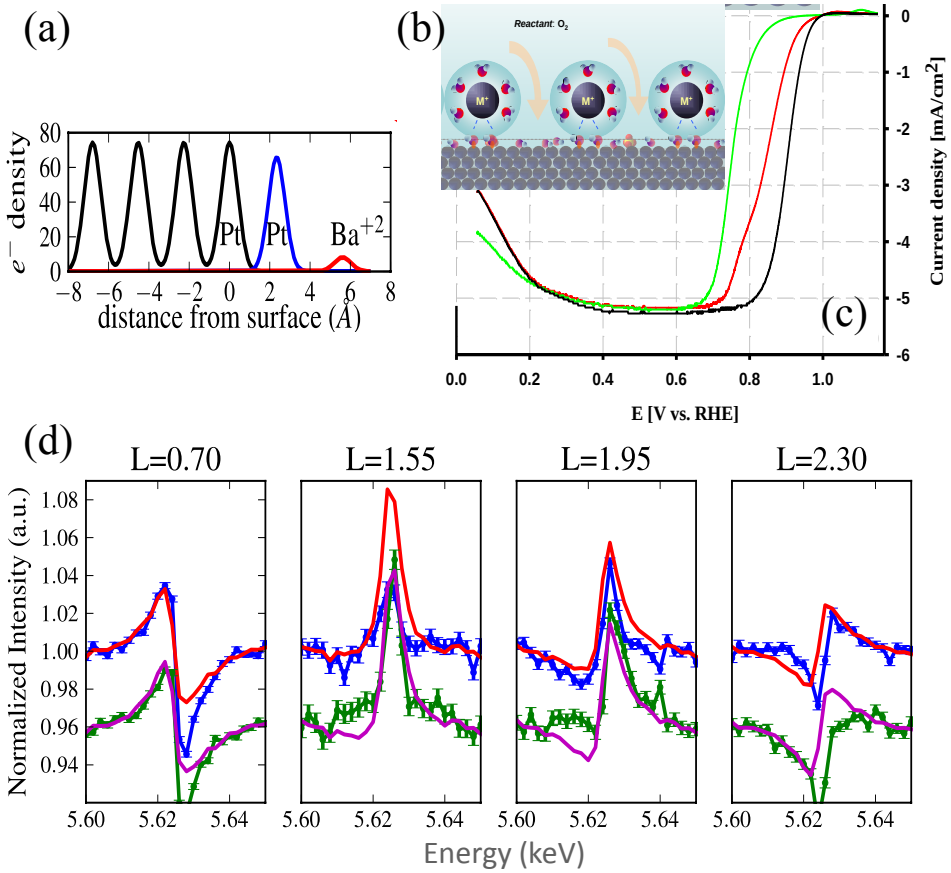
Pt(111)



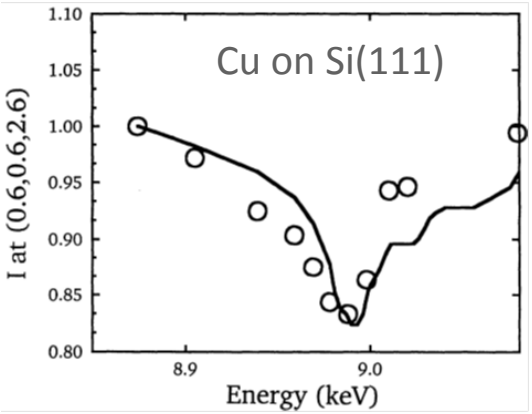


Physica B 283 212 (2000)

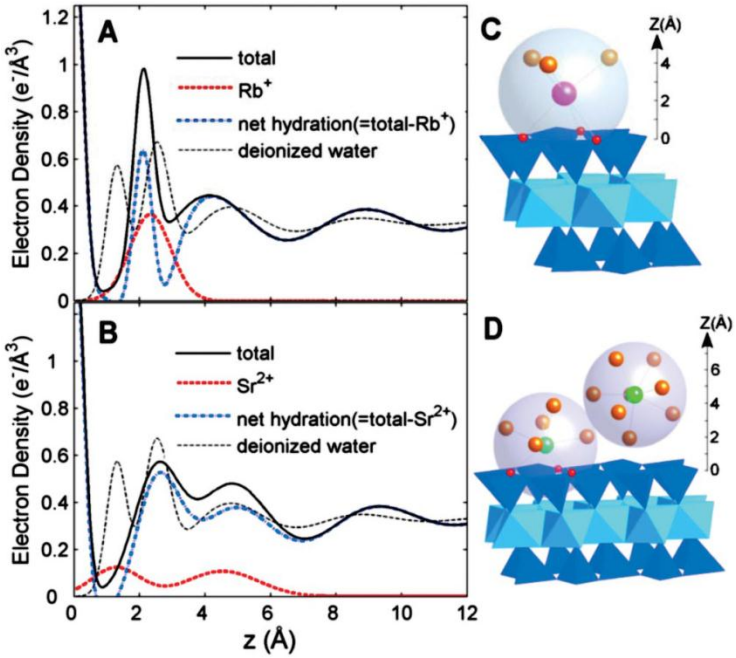
Foreign Atoms on Surface



Strmcnik, Chang, et al., Phys. Chem. Lett., 2011



Walker, Specht, McKee, PRL 1991



Park, Fenter et al., PRL 2006

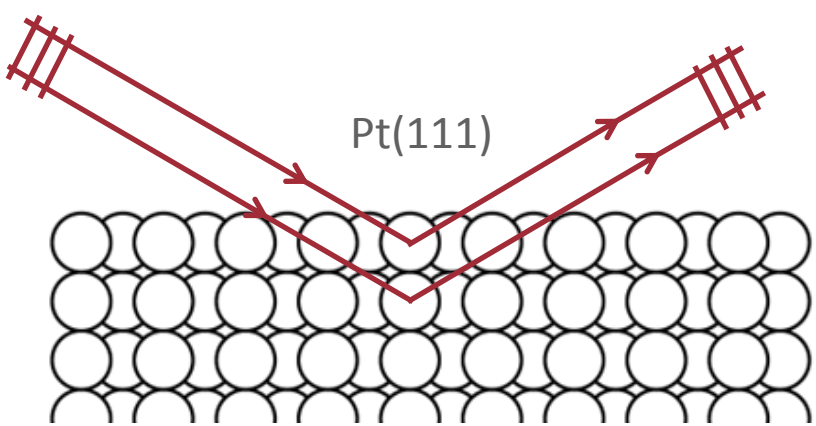
Same Atom with Different Chemical State

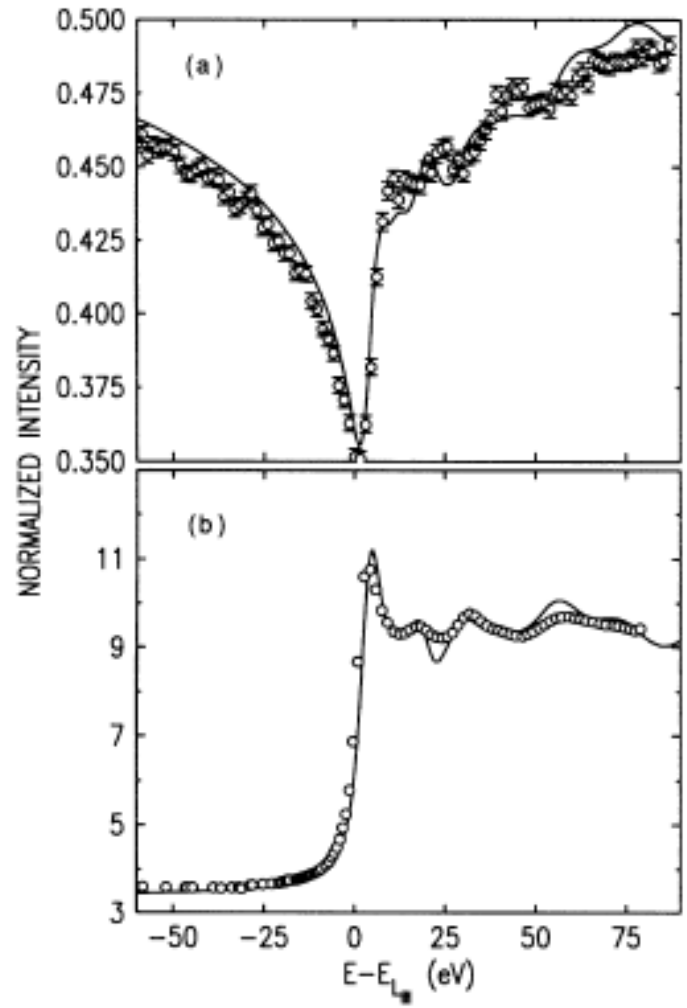
$$S(L,E) = f^1{}_{Pt}(L,E) + f^2{}_{Pt}(L,E)e^{-i2\pi L} + f^3{}_{Pt}(L,E)e^{-2i2\pi L} + \cdots$$

$$= f^1{}_{Pt}(L,E) + f_{Pt}(L,E)\left(e^{-i2\pi L} + e^{-2i2\pi L} + \cdots\right)$$

$$= f^1{}_{Pt}(L,E) + f_{Pt}\sum_{n=1} e^{-ni2\pi L}$$

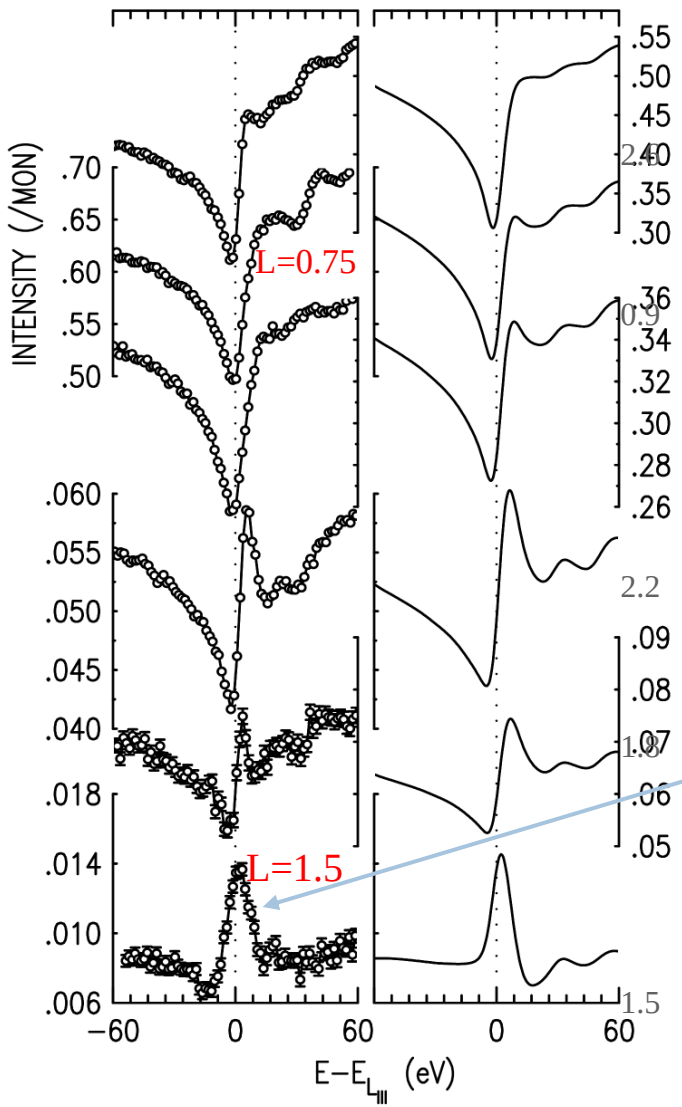
$$= f^1{}_{Pt}(L,E) + \frac{f_{Pt}e^{-i2\pi L}}{1 + e^{-ni2\pi L}}$$

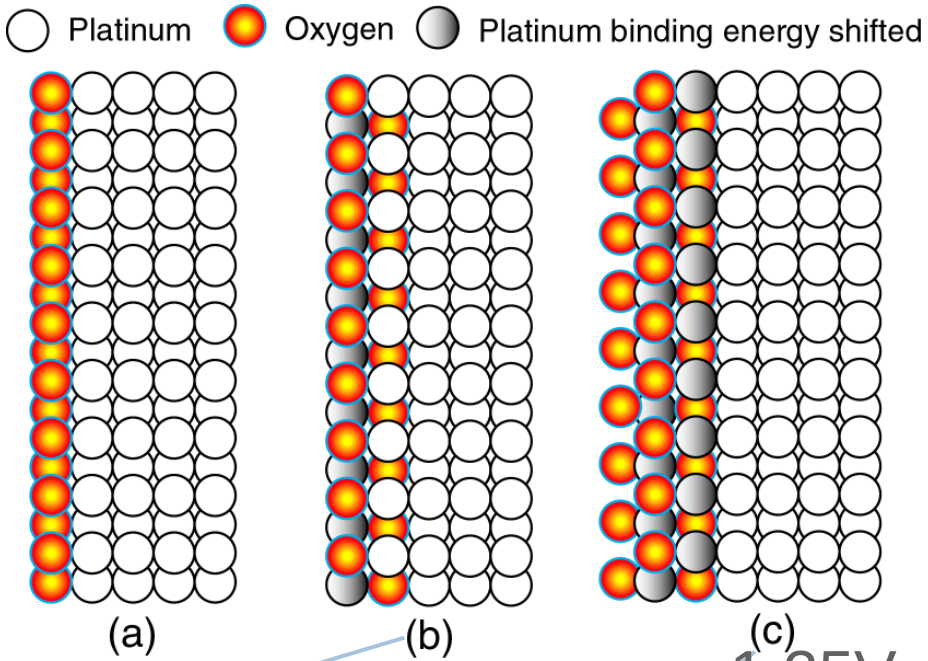




Physica B 283 212 (2000)

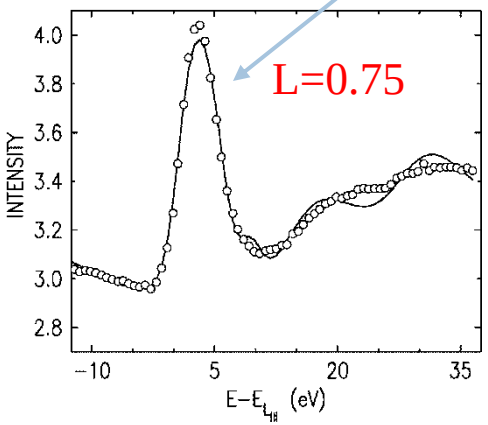
Anomalous Peak-like Resonance Scattering at L=1.5 and 0.75





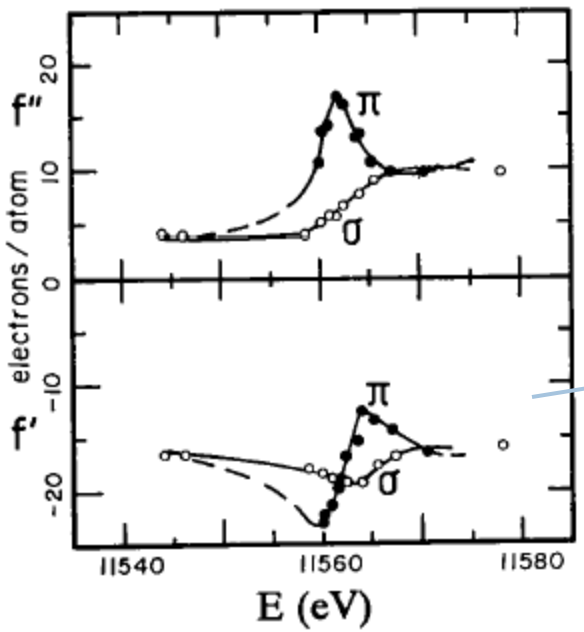
1.05V

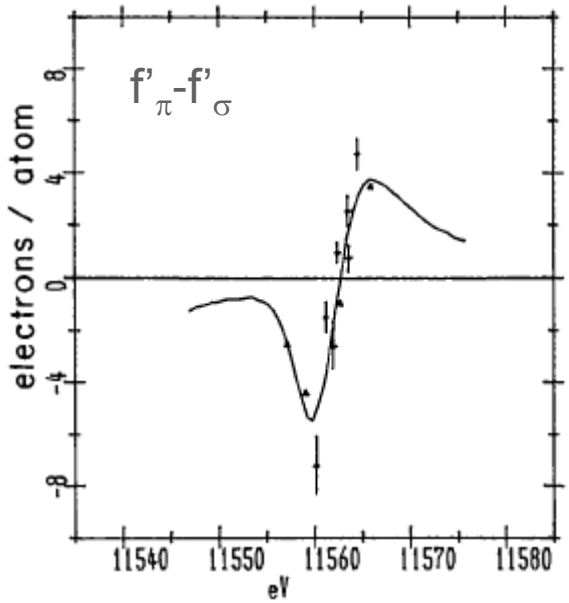
1.25V



Y. Chu, et al., PRL 83, 552 (1999)

Templeton-Templeton Scattering

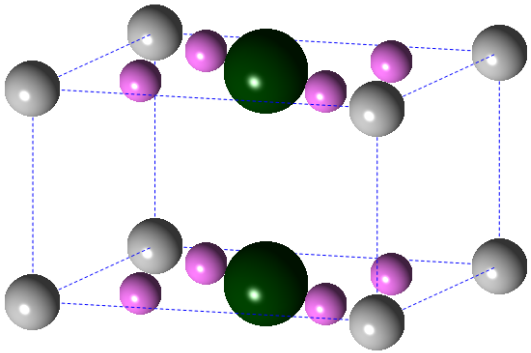




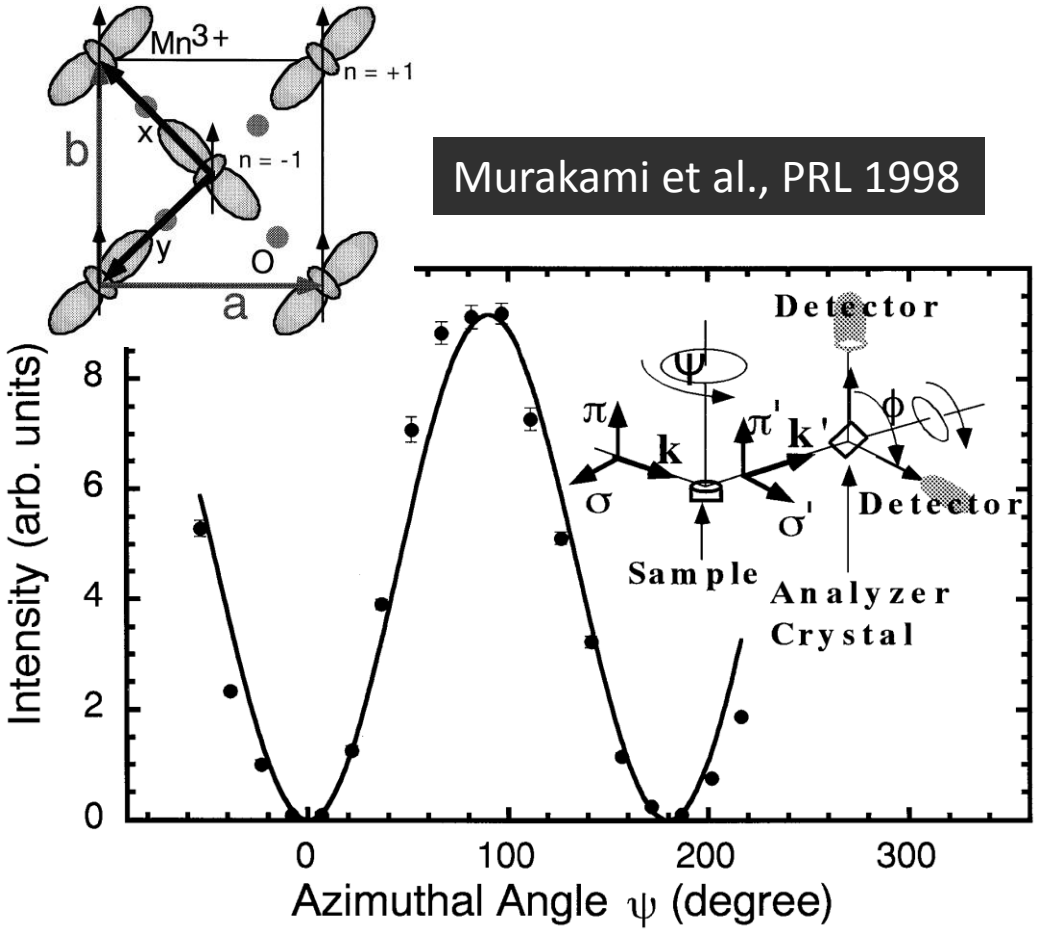
Templeton and Templeton,

Acta Cryst. (1985). **A41**, 365–371

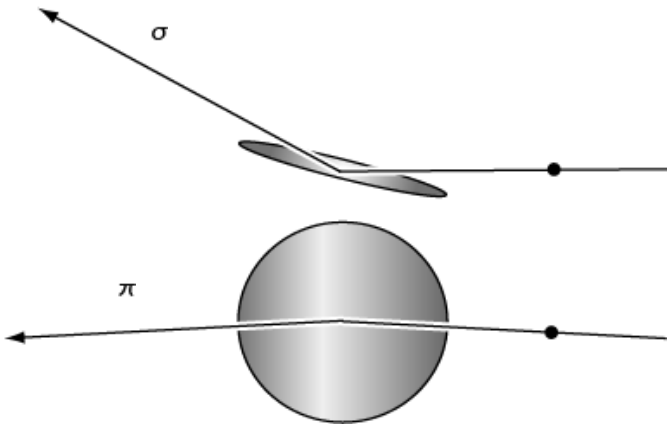
K_2PtCl_4
P4/mmm
a=7.023A
c=4.149A
Pt:0,0,0
Cl:x,x,0; x=0.23
K:.5,.5,0



Orbital Ordering in $LaMnO_3$



Polarization Dependence: Surface Templeton Scattering

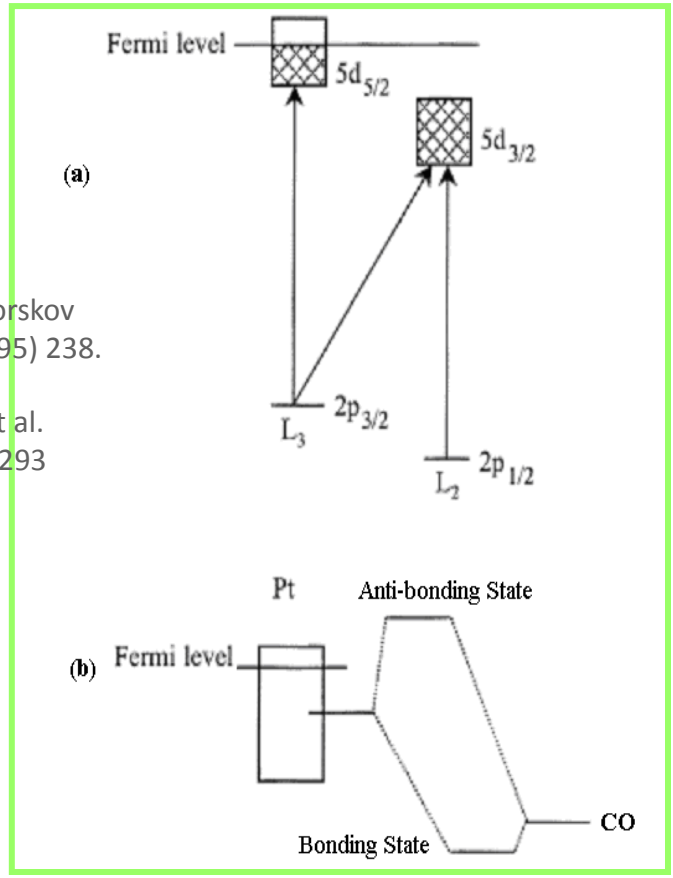


Surface Resonance X-ray Scattering: Polarization Dependence

$$
\begin{aligned}
&(e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}\cdot\boldsymbol{\varepsilon})_{I_{CO}L_{III}} \\
&= im\omega \int d\phi\, dz\, d\rho\rho\, \Phi_{L_{III}} Z_{L_{III}} \Gamma_{L_{III}} \\
&\quad \times [e^{ik_\rho \rho\cos\phi} e^{ik_z z}(\varepsilon_\rho \rho\cos(\phi-\pi/2) + z\varepsilon_z)] \\
&\quad \times \Phi_{CO} Z_{CO}(z - z_{CO}) \Gamma_{CO} \\
&= im\omega\varepsilon_\rho \int d\phi\, \Phi_{L_{III}} \Phi_{CO} \\
&\quad \times \int d\rho\rho\, \Gamma_{L_{III}} \Gamma_{CO} [e^{ik_\rho \rho\cos\phi} \rho\cos(\phi-\pi/2)] \\
&\quad \times \int dz\, Z_{L_{III}} [e^{ik_z z}] Z_{CO}(z - z_{CO}) \\
&\quad + im\omega\varepsilon_z \int d\phi\, \Phi_{L_{III}} \Phi_{CO} \\
&\quad \times \int d\rho\rho\, \Gamma_{L_{III}} \Gamma_{CO} [e^{ik_\rho \rho\cos\phi}] \\
&\quad \times \int dz Z_{L_{III}} [e^{ik_z z} z] Z_{CO}(z - z_{CO})
\end{aligned}
$$

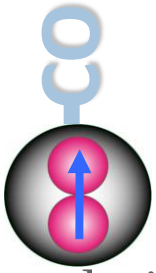
Hammer and Norskov
Nature, **376** (1995) 238.

D. E. Ramaker, et al.
PCCP, 1 (1999) 2293

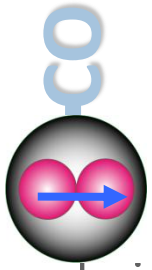


Pt $2p_{3/2} \rightarrow$ CO $2\pi^*$

Sensitive to CO Bond Direction.

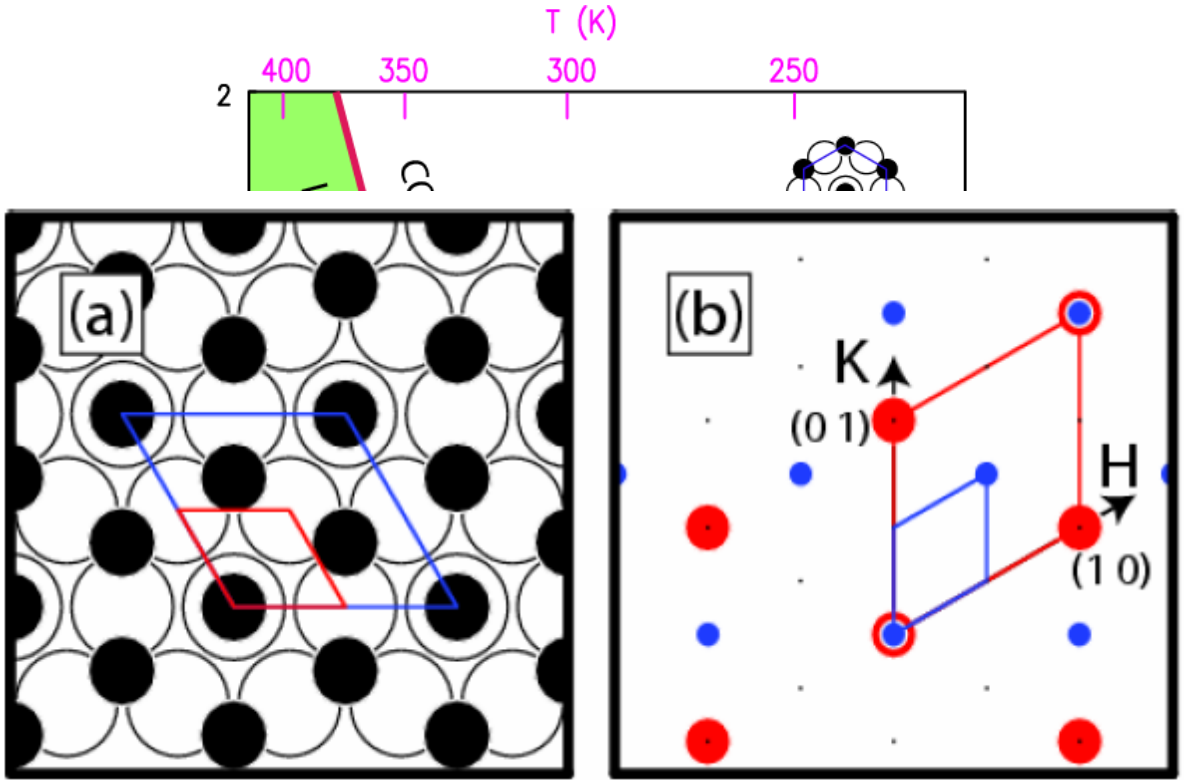


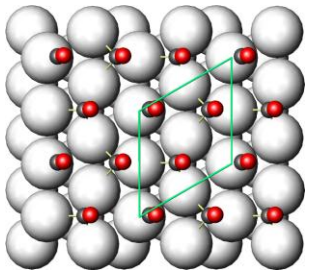
p-polarization

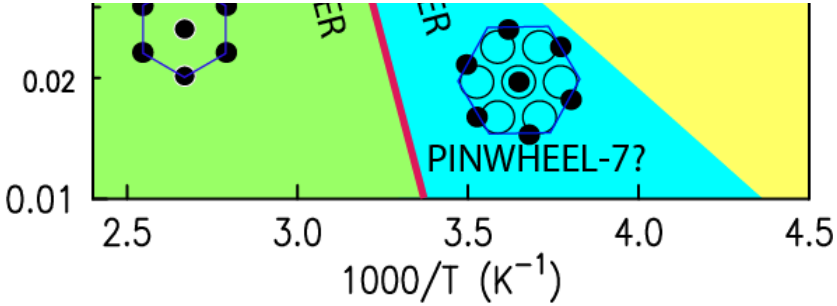


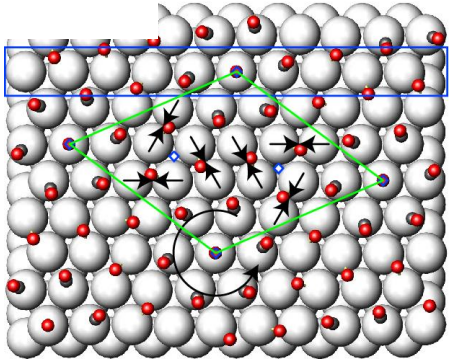
s-polarization

Structures of Electrosorbed CO on Pt (111)



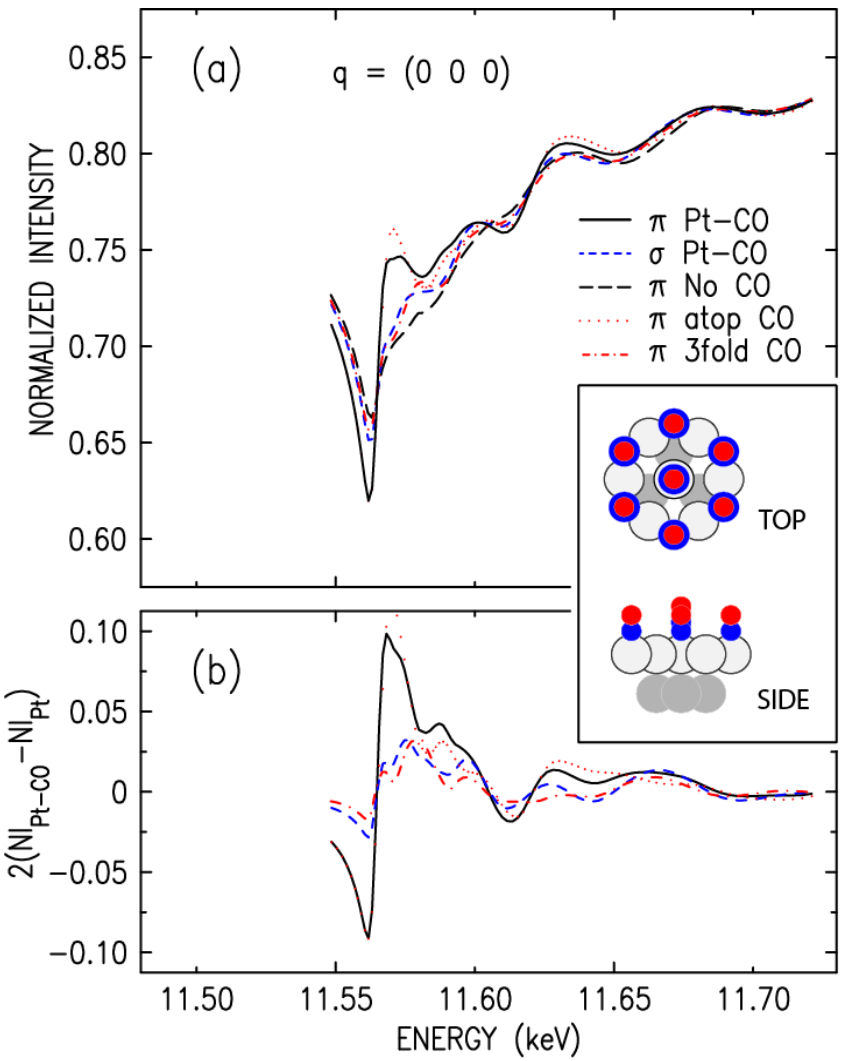


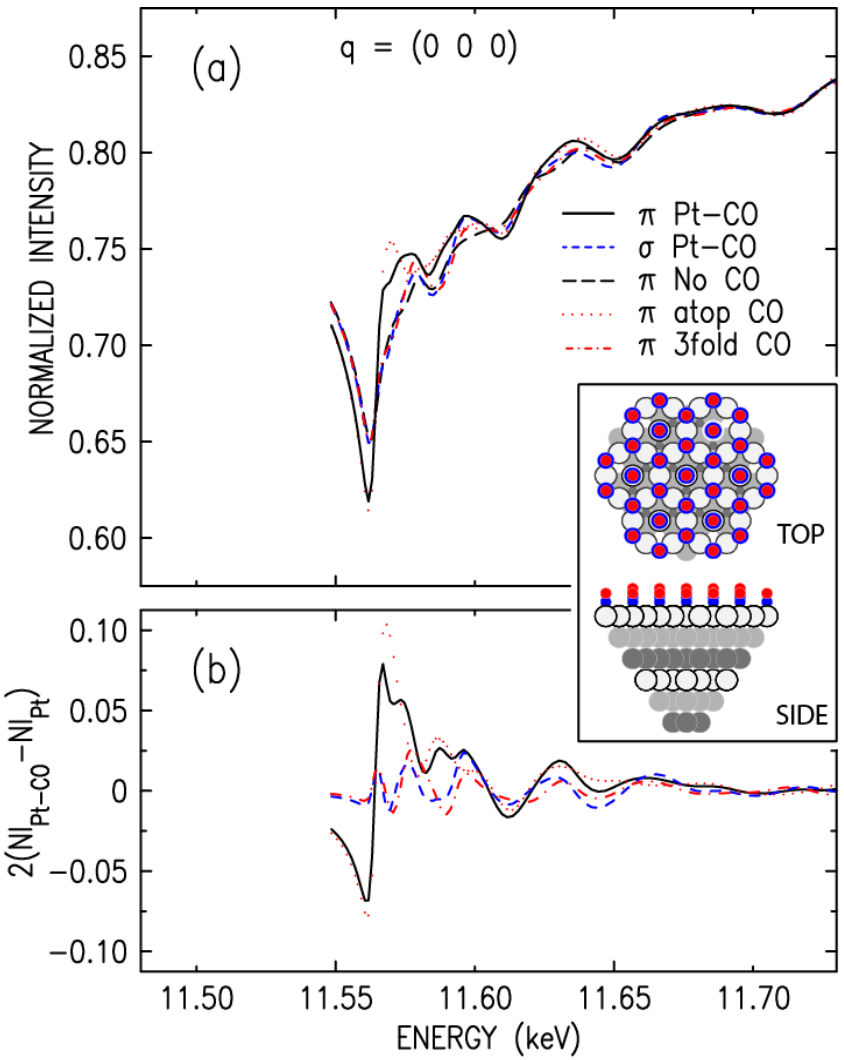




Menzel, Chang, Komanicky, Tolmachev, Tkachuk, Chu, You, Phys. Rev. B75, 035426 (2007)
Chang, Menzel, Komanicky, You, Electrochimica Acta, 52, 5749 (2007)

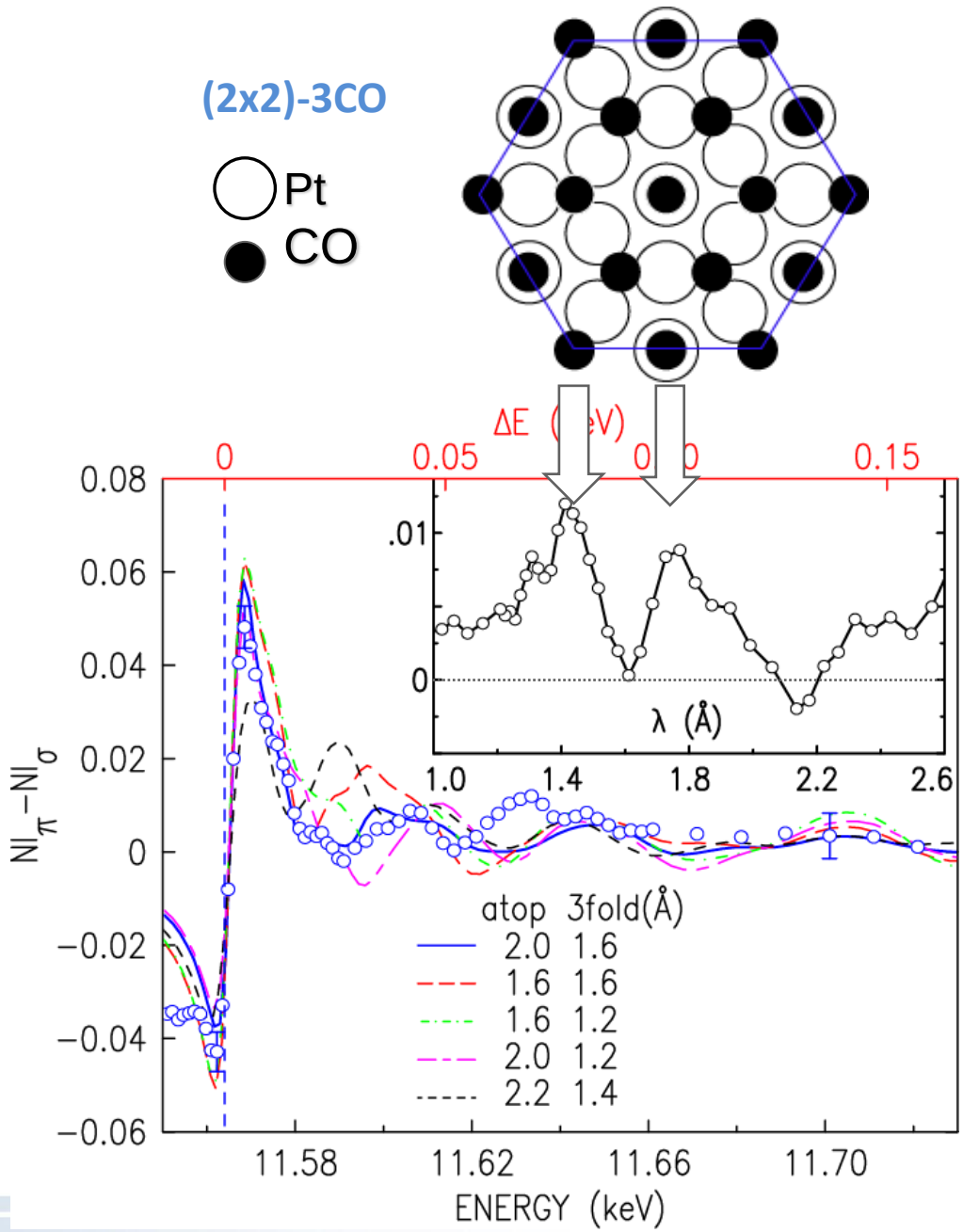
FEFF8


(a)
q = (0 0 0)
NORMALIZED INTENSITY
0.85
0.80
0.75
0.70
0.65
0.60
π Pt−CO
σ Pt−CO
π No CO
π atop CO
π 3fold CO
TOP
SIDE
(b)
2(NI_Pt−CO − NI_Pt)
0.10
0.05
0
−0.05
−0.10
11.50
11.55
11.60
11.65
11.70
ENERGY (keV)

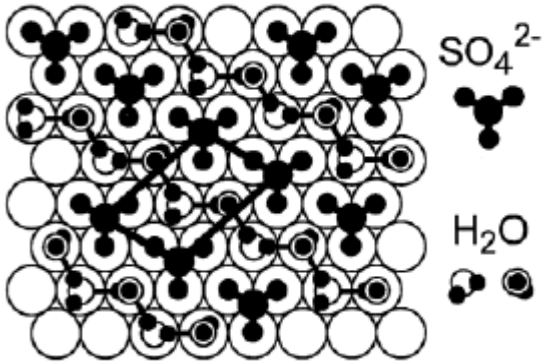

(a)
q = (0 0 0)
NORMALIZED INTENSITY
0.85
0.80
0.75
0.70
0.65
0.60
π Pt−CO
σ Pt−CO
π No CO
π atop CO
π 3fold CO
TOP
SIDE
(b)
2(NI_Pt−CO − NI_Pt)
0.10
0.05
0
−0.05
−0.10
11.50
11.55
11.60
11.65
11.70
ENERGY (keV)

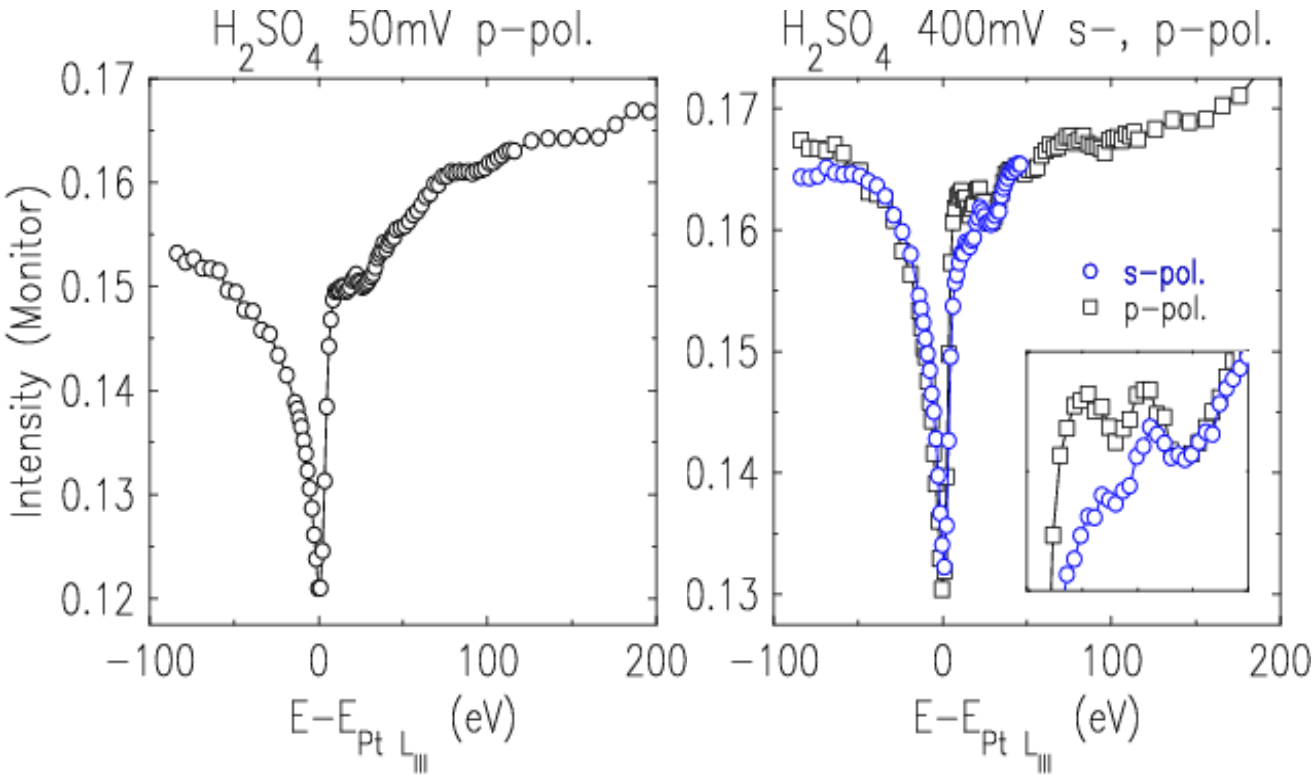
Polarization-Dependent Resonance Anomalous Surface Scattering

Menzel, Tolmachev, Chang, Komanicky, Chu, Rehr, You Europhys. Lett. 74 (2006) 1032.

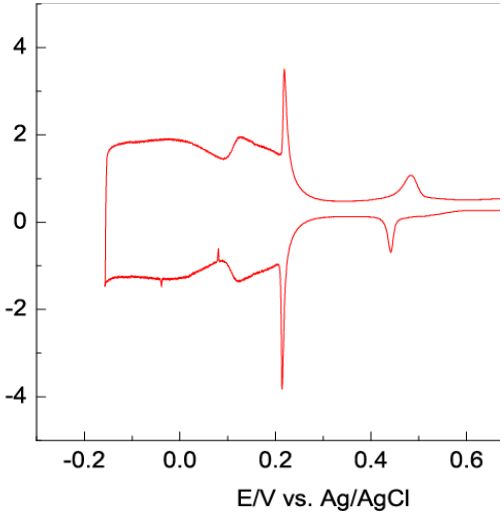


Sulfate Adsorption

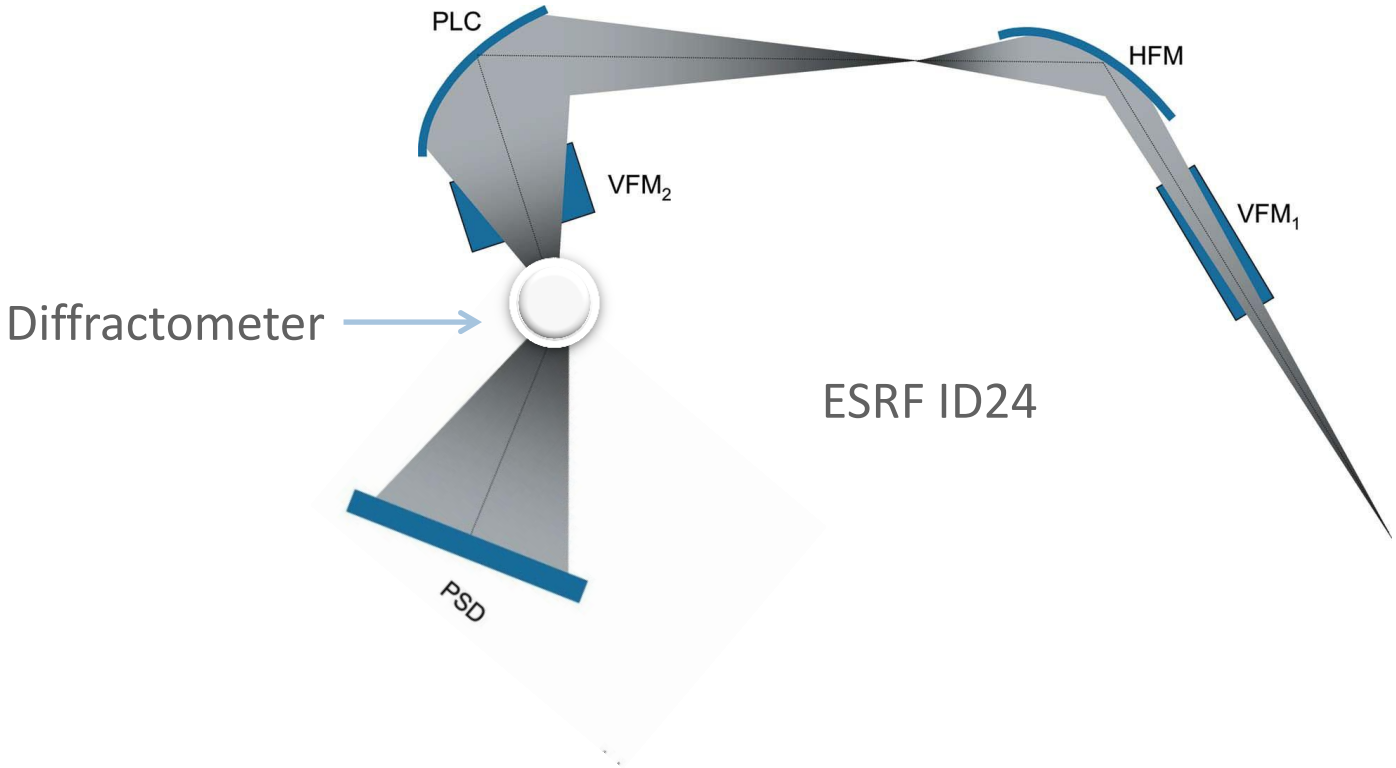




Funtikov, *et al*. J. Electroanal. Chem. 428, 147 (1997).



Energy-Dispersive Setup



Pascarelli, et al., J. Synch. Rad. 2006