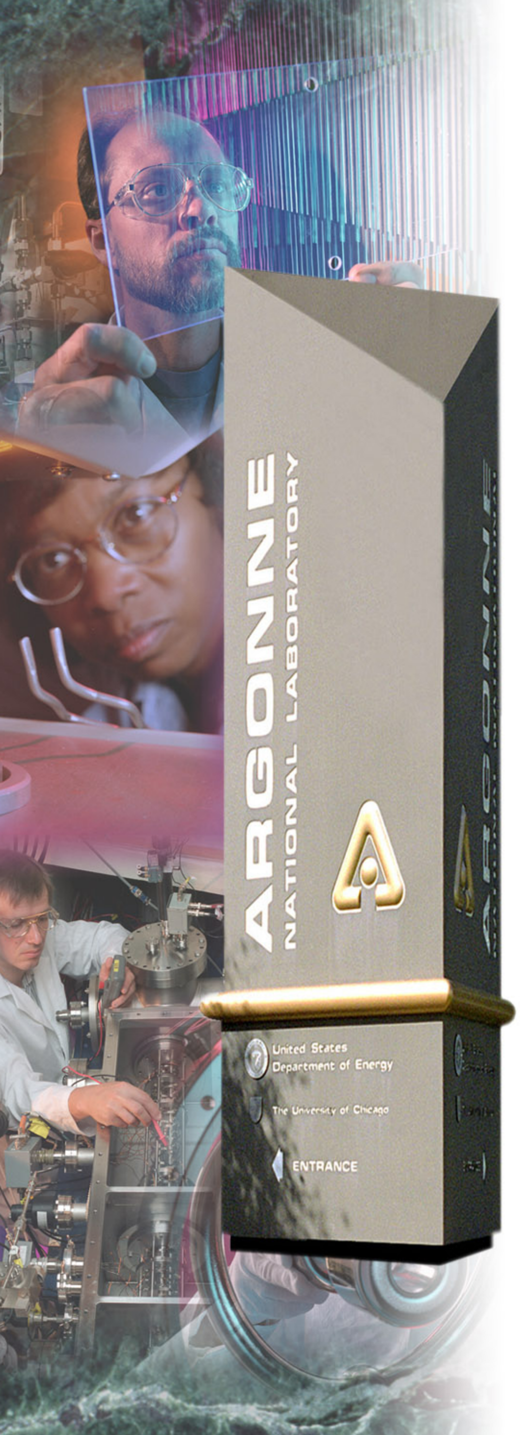


Resonant X-ray Scattering

Michel van Veenendaal
Advanced Photon Source,
Northern Illinois University

Office of Science
U.S. Department of Energy

A U.S. Department of Energy
Office of Science Laboratory
Operated by The University of Chicago

Synchrotron-Related Theory

SRT is a joint program between Northern Illinois University and the Advanced Photon Source

Two permanent staff members:
Michel van Veenendaal (NIU/ANL)
Roland Winkler (NIU/ANL)

Two postdocs (three from 1/2006):
Ken Ahn (APS)
Serkan Erdin (NIU)

parttime: Art Fedro (Prof. Emeritus NIU)

http://www.aps.anl.gov/Experimental_Facilities_Division/Synchrotron_Related_Theory

NORTHERN ILLINOIS UNIVERSITY

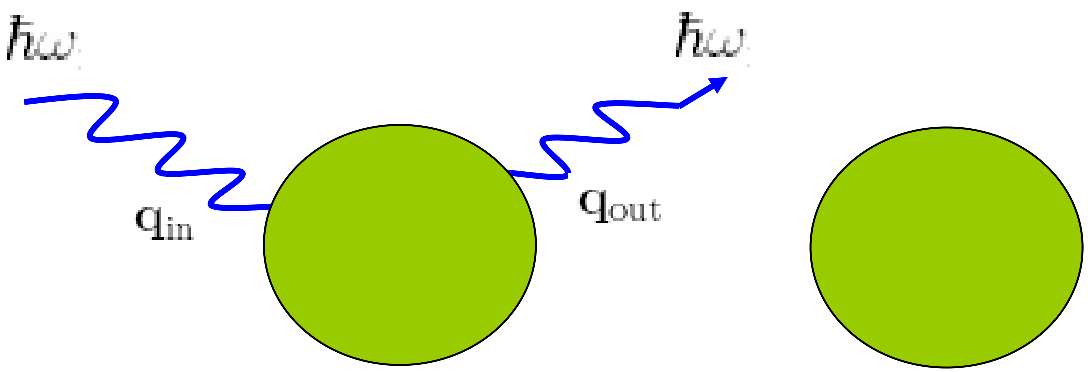
Advanced Photon Source

Why theory?

- Provide theoretical support for experimental program at the APS
- Establish a link between experiment and theoretical models
- Independent theory to create pathways to new experiments
- Inspire experimentalists to look in new and exciting directions

X-ray Scattering

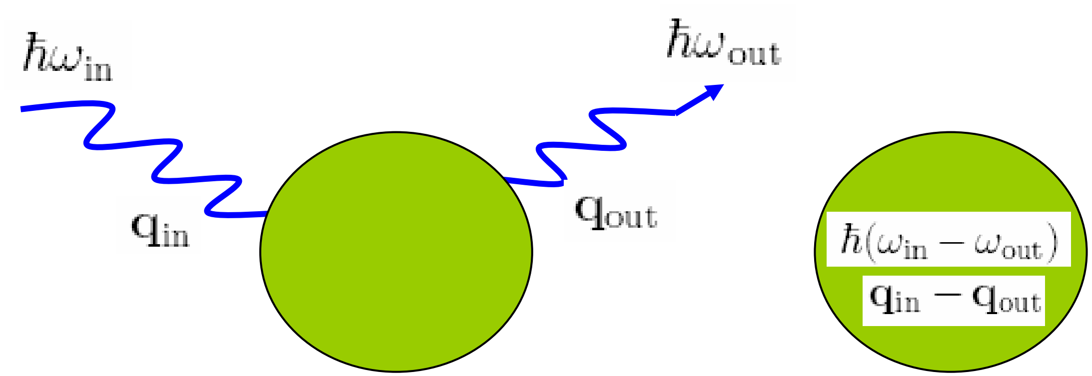
Elastic X-ray Scattering



Structure:

crystal structure
magnetic structure
orbital ordering

Inelastic X-ray Scattering



Excitations:

Charge, magnetic,
collective excitations,
phonons,
structure factors

Resonant X-ray Scattering

Make use of a certain core-level

Transition metals: 2p→3d (500-1000 eV), 1s →4p (several keV), 3p→3d (tens of eV)

Rare earths: 3d→4f (800-1500 eV), 2p→5d (several keV).

Advantages: chemically selective, sensitive to magnetic and orbital ordering

How does $Nd_2Fe_{14}B$, one of the strongest magnets, work?

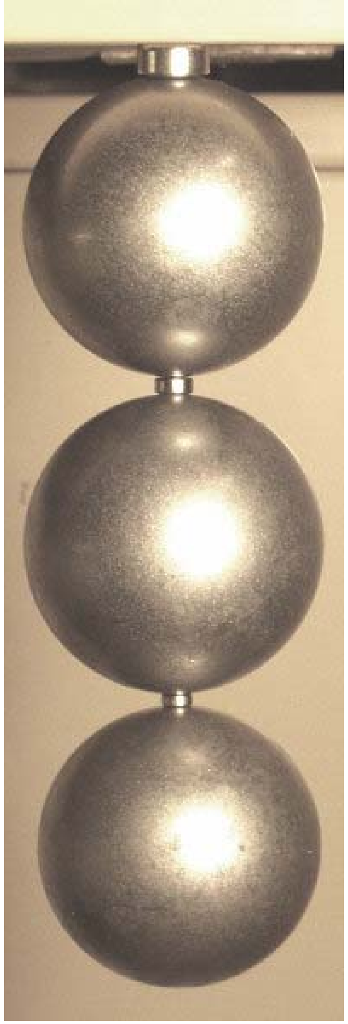
Coercivity: the magnetic field need to reduce the magnetization of a fully saturated sample to zero

Fe_3O_4 magnetite

Sintering and defect pinning

$Nd_2Fe_{14}B$

Interaction between the iron (Fe) and the rare-earth ions (Nd)



D. Haskel, J. C. Lang, Z. Islam, A. Cady, G. Srajer,

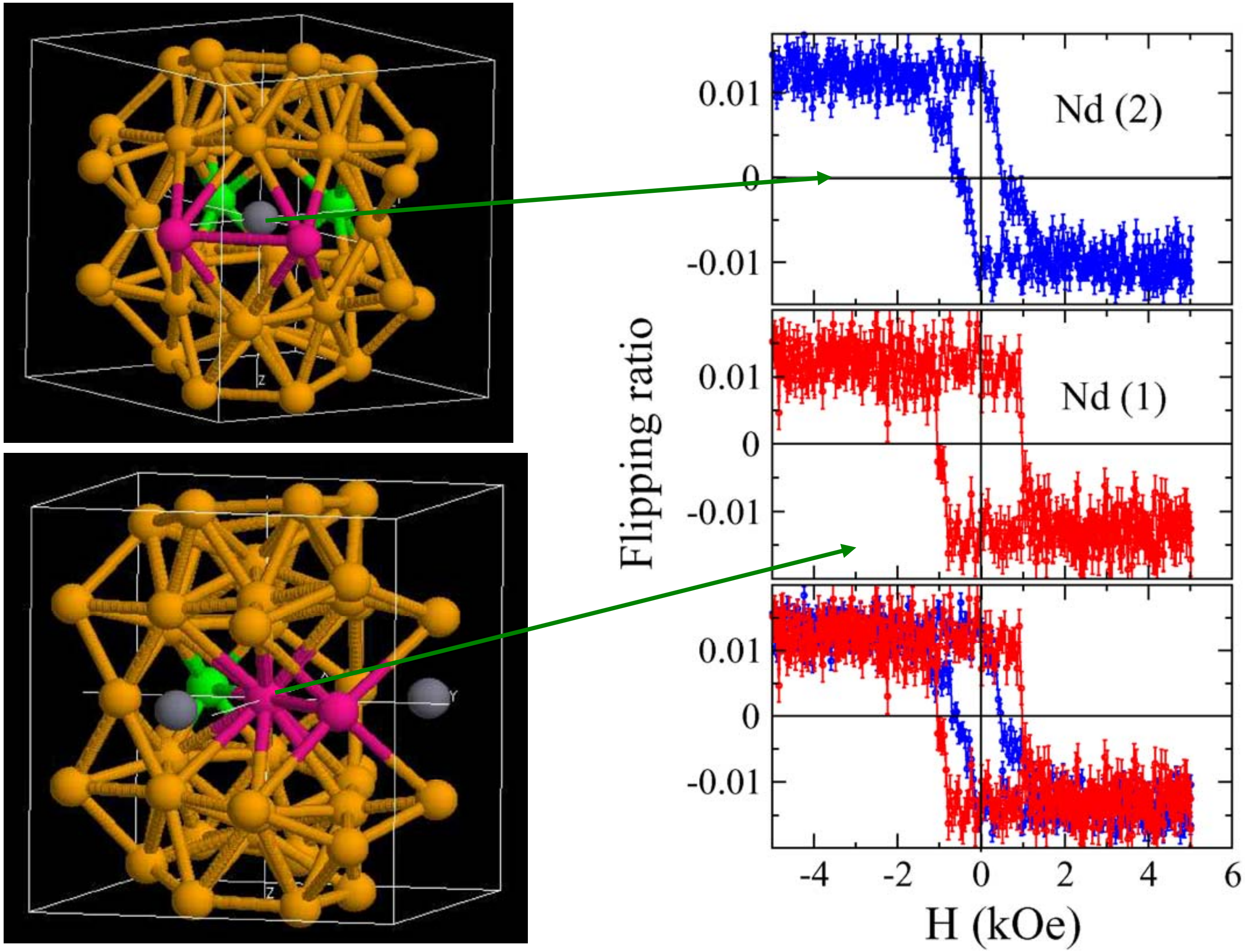
M. van Veenendaal, P. C. Canfield

accepted for publication in Phys. Rev. Lett.

Nd site-specific hysteresis loops

Use two diffracting conditions to separate Nd(1) and Nd(2) magnetic sites

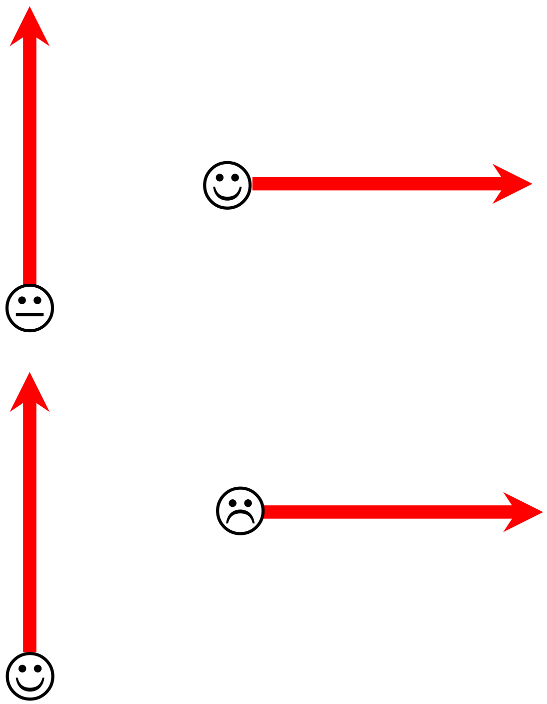
- Nd (1)
- Nd (2)
- B
- Fe

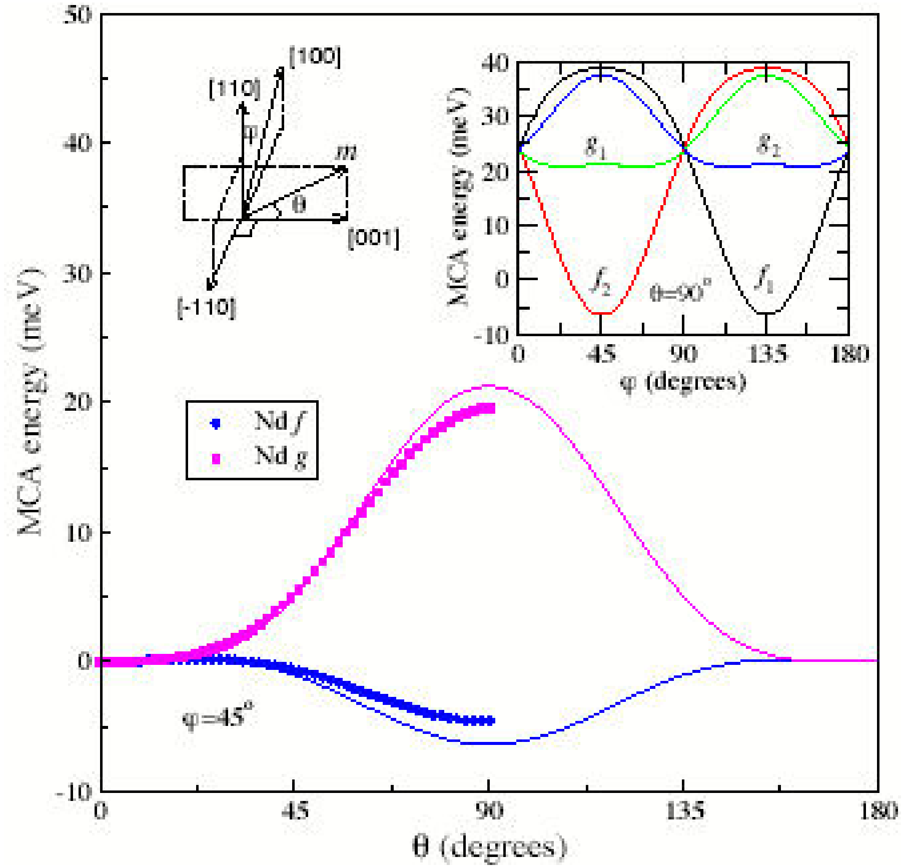


Magnetic moments on different Nd sites

f

g

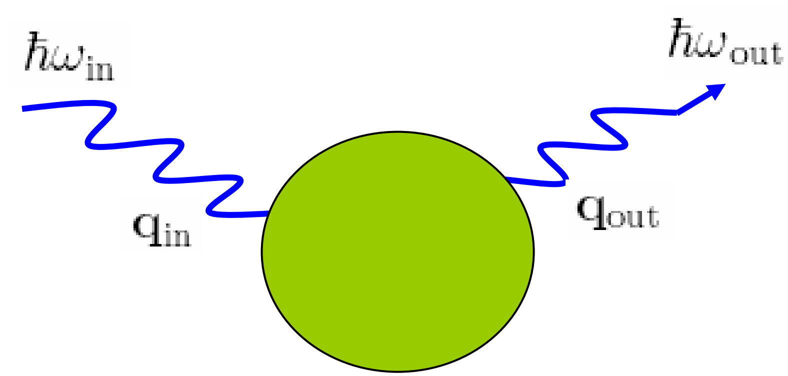


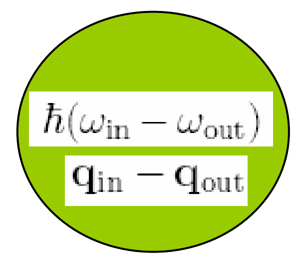


θ= 0 90 degrees

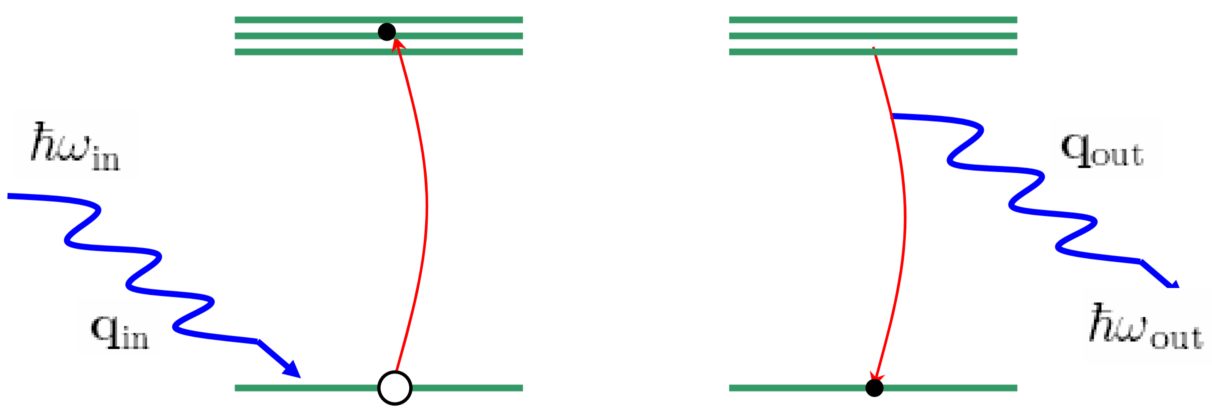
Resonant Inelastic X-ray Scattering

Inelastic X-ray Scattering





Resonant Inelastic X-ray Scattering



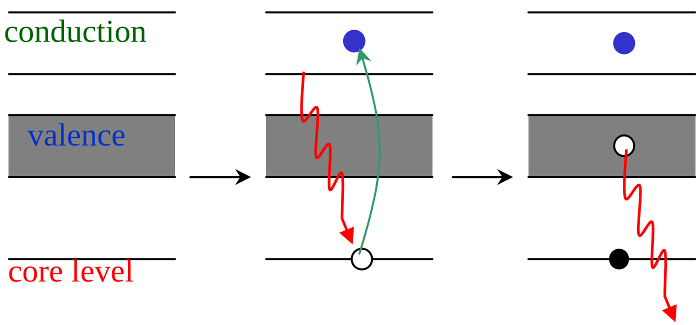
Electronic excitations:
Charge, magnetic, collective excitations

Pro and Cons of RIXS

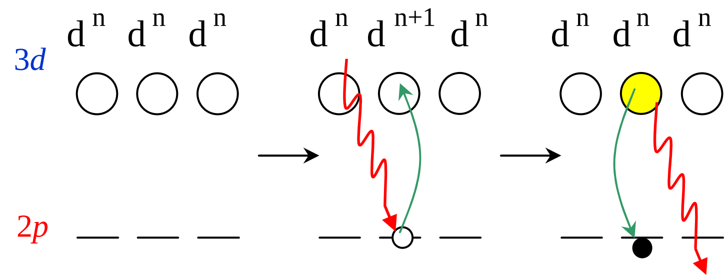
- **Bulk sensitive**
- **Chemically selective, but without core hole in final state**
- **Measures q,ω dependent valence excitations**
- **Low cross section (even with enhancement)**
- **Interpretation not trivial**

Not all RIXS's are created equal

(a) RIXS in semiconductors

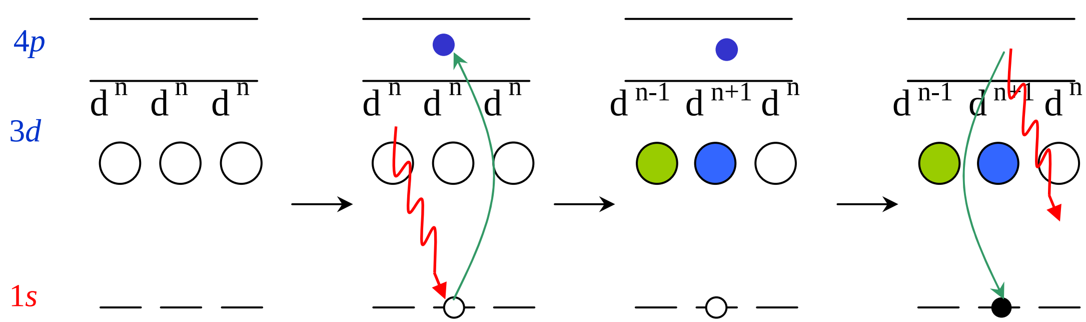


(b) *L*-edge RIXS in transition-metal compounds



XAS intermediate state

(c) *K*-edge RIXS in transition-metal compounds

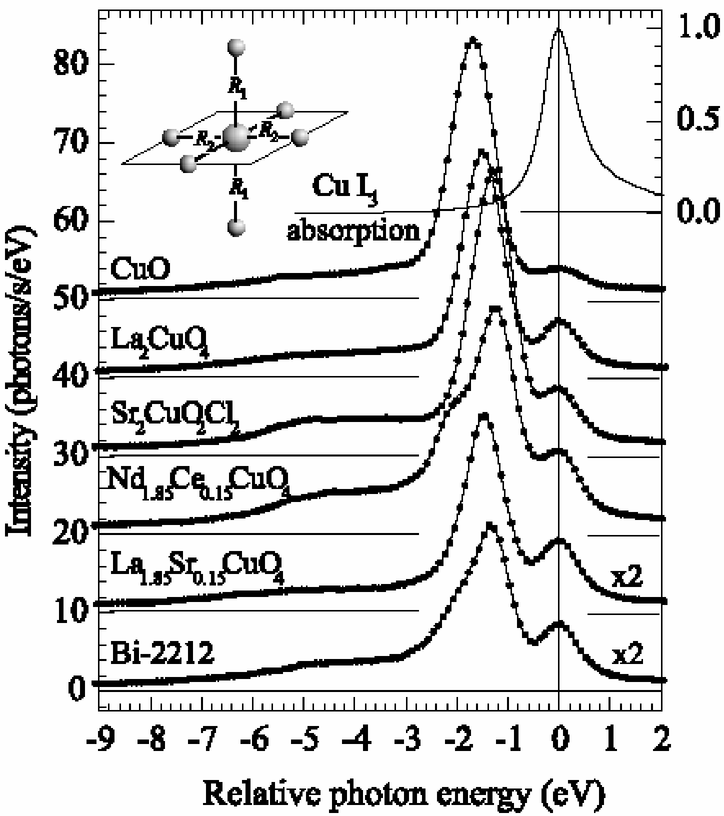


"XPS" intermediate state
=>Satellite structures

VOLUME 92, NUMBER 11 PHYSICAL REVIEW LETTERS week ending 19 MARCH 2004

Low Energy Electronic Excitations in the Layered Cuprates Studied by Copper L_3 Resonant Inelastic X-Ray Scattering

G. Ghiringhelli,[1] N. B. Brookes,[2] E. Annese,[3] H. Berger,[4] C. Dallera,[1] M. Grioni,[5] L. Perfetti,[5] A. Tagliaferri,[1] and L. Braicovich[1]



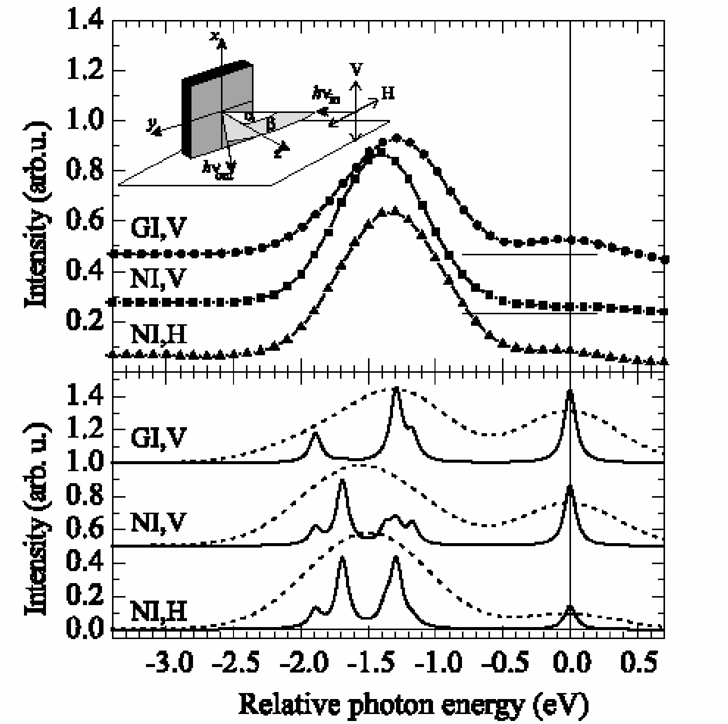
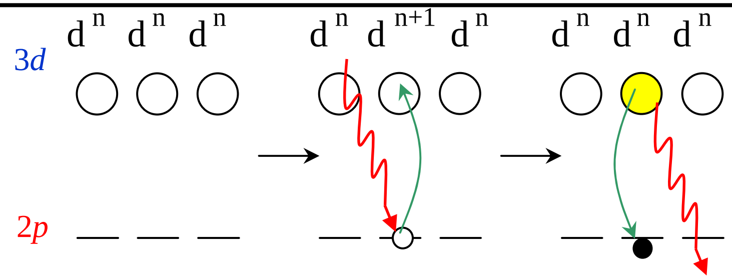
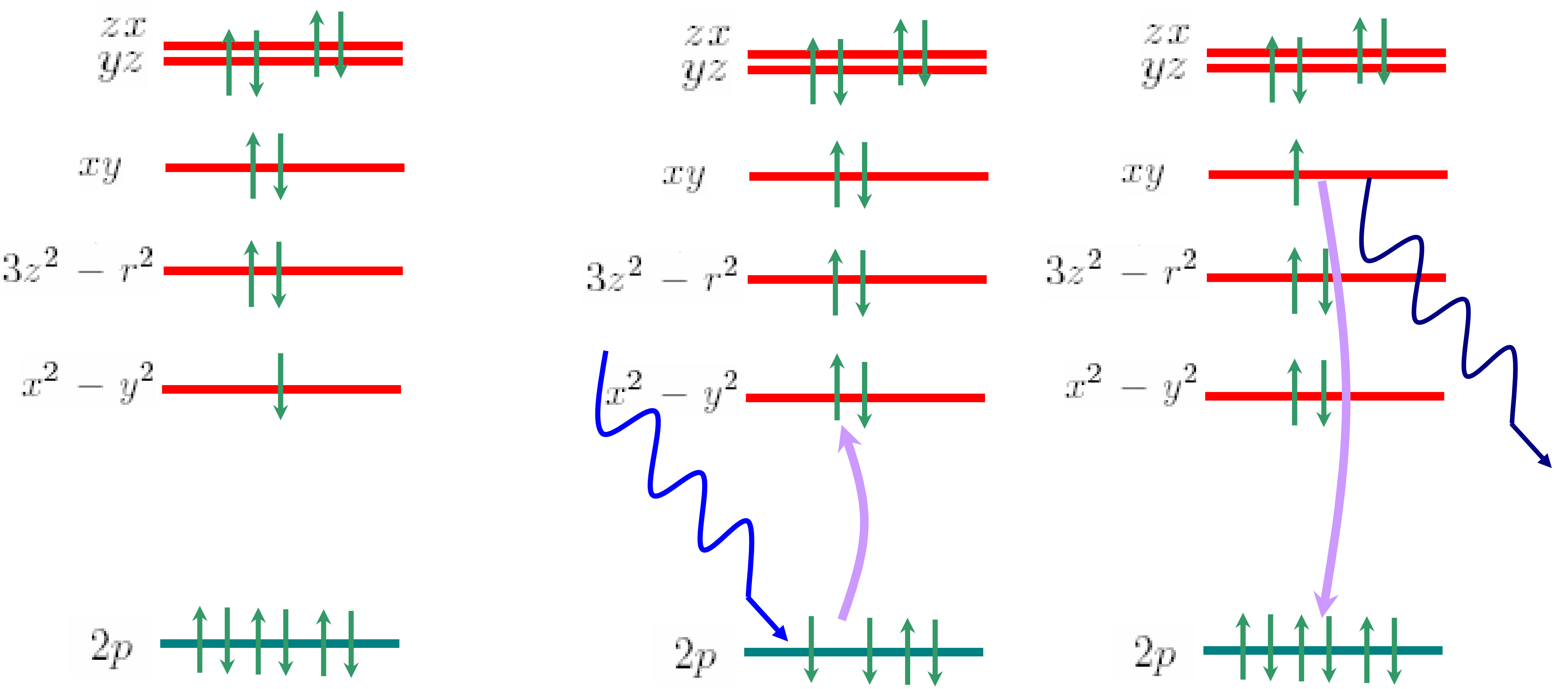


FIG. 3. Upper panel: RIXS spectra of $Sr_2CuO_2Cl_2$ measured at grazing and normal incidence with V and H polarizations ([GI,V], [NI,V], [NI,H]). Bottom panel: calculated spectra for the same scattering geometries. Inset: experimental geometry, where $\beta = 70°$ is the scattering angle and $\alpha = 0°$ (80°) is the incidence angle in the NI (GI) configuration.

L or *M*-edge RIXS in transition-metal compounds

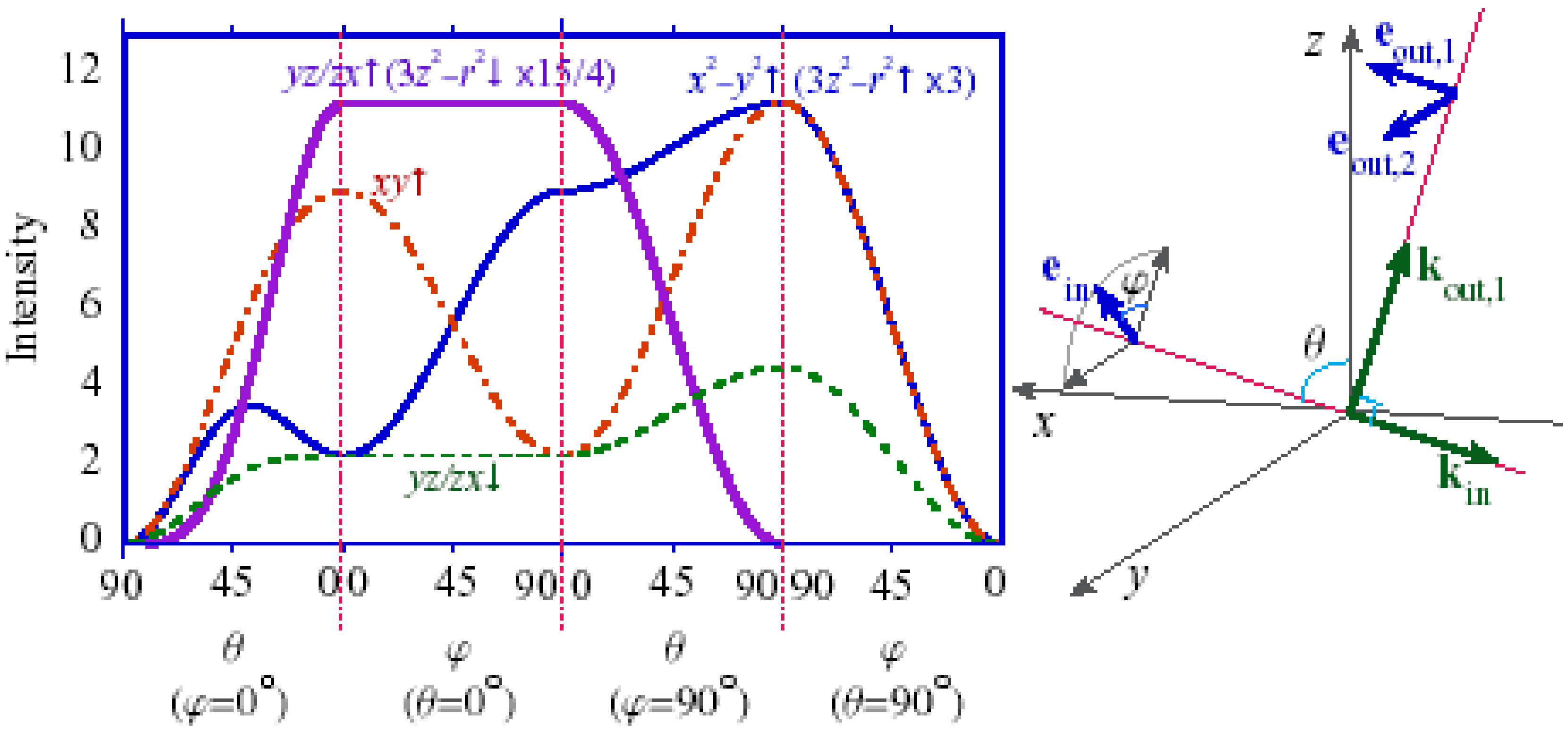
Simplest example:





Exact Solutions

- Strength zero-loss line
- Spin-flip processes or single magnon excitations
- Detailed angular and polarization dependencies



RIXS on Cu^{2+} ion

- Strong dependence of spectral weights
- No spin flip