INSTITUTO DE FÍSICA GLEB WATAGHIN

PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA

1º SEMESTRE DE 2024

FI229 – Tópicos Física Aplicada III – "Topics in core level spectroscopy: Theory and simulations."

A disciplina será ministrada em inglês.

Turma
A

Créditos
2

Horário
Quarta – 8h às 10h na sala IF15

Docente
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I Introduction

X-ray excitations of core electrons in solids, combined with a sensitive measurement of its effects, can give information about the local crystal and electronic structure, nature of bonding between ions (i.e., angle or length bonding), etc. This can be carried out using synchrotron radiation sources that allow the performance of different techniques which are known as core-level spectroscopies. Some examples are XAS (X-ray absorption spectroscopy), RIXS and REXS (Resonant inelastic and elastic X-ray scattering), nIXS (non-resonant inelastic X-ray scattering), XPS (X-ray photoelectron spectroscopy), etc. The physical interpretation of the obtained experimental data from such spectroscopies usually demands an elaborated theoretical framework and related computational tools. This guide course gives the student fundamental concepts about the current theoretical approaches used to interpret experimental data obtained from the core-level spectroscopies. The objective is that the student can calculate different core level spectroscopy types on solids using the free software Quanty, a quantum many body script language designed for such a purpose. Other software as CTM4DOC and Crispy, which are graphic user interfaces for Quanty, will be used as well. Finalizing this course it is expected that the student can calculate different X-ray spectroscopy for $BiFeO_3$ and rare earth nickelates $RNiO_3$ (R = Sm, Nd, and La), which are the materials synthesized at the nanomagnetism laboratory and have been studied experimentally by the group under different core-level spectroscopies at synchrotrons.

II Objectives

The aims of the course are:

- Show theoretical models currently employed to analyze the core-level spectroscopies in solids.
- Model different types of X-ray spectroscopy using the free-software Quanty, CTM4DOC and Crispy for different materials.
- Give the needed theoretical and computational skills to calculate X-ray spectroscopy in functional materials (based on transition metal oxides) to analyze the experimental results obtained with BiFeO3 and RNiO3, which has been synthesized at the nanomagnetism laboratory and studied under synchrotron radiation.

III Skills to be developed

The student who completes this guide course should:

- Know and understand all the core-level spectroscopy techniques.
- Understand different ab initio many-body techniques (and their limitations) employed to calculate different types of X-ray spectroscopy.
- Employ the multiplet charge-transfer theory to calculate X-Ray spectroscopies (XAS, XMCD, REXS, RIXS and XPS) in different solids using the software Quanty.
- Calculate XAS and XPS for different solids using CTM4DOC and Crispy software.
- Employ Quanty and basics of DFT (Density functional theory) to analyze experimental measurements of XAS, XMCD and REXS performed on BiFeO3 and RNiO3.

IV Proposed weekly schedule

Week	Topic	Quanty Tutorial	Homework
1	Introduction to core level spectroscopy	Tutorial #1: Quanty installation and first steps	-
2	X-Ray Fluorescence (XRF)	-	Homework #1: Introduction and XRF
3	Linear response theory	Tutorial #2: XRF Simulations, Basic spectrum simulation	-
4	Experimental tools	-	Homework #2: Linear response and Tools
5	X-Ray Photoelectron Spectroscopy (XPS)	Tutorial #3: Simulations with different tools and devices, XPS Simulations	-
6	X-Ray Absorption Spectroscopy (XAS)	-	Homework #3: XPS and XAS
7	Electron-electron interactions	Tutorial #4: XAS Simulations, Modeling systems with strong interactions	-

8	Integrated Case Studies: Batteries, Catalysts, Heterostructures and interfaces, Magnetic Materials	-	Homework #4: Integrated case stud-ies
9	**Break - 30%**	-	-
10	Valence and core electron resonance	Tutorial #5: Resonance spectrum modeling	-
11	Spectroscopy in low dimensionality systems	-	Homework #5: Low dimensionality
12	Correlations and magnetism	Tutorial #6: Simulations in a selected correlated system (1D and 2D)	-

Week	Topic	Quanty Tutorial	Homework
13	X-Ray Magnetic Circular Dichroism (XMCD) and related techniques	-	Homework #6: XMCD and applications
14	Disordered systems and liquids	-	Homework #7: Disordered systemsand Advanced techniques
15	Advanced techniques in spectroscopy	Exploration of advanced features	-
16	**Review**	General review	**Final Assessment**

V Metodology

Graduate level (4 credits): The course will include weekly lectures complemented by tutorials and example codes as specified in the syllabus. As the course progresses, the complexity of spectroscopy calculations and their associated theory will increase. The objective is to introduce students to the correct physics of electron-correlated materials within the framework of many-body physics. In the concluding weeks, graduate students will be required to undertake a final project, applying the principles of core-level spectroscopy to materials relevant to their thesis research.

VI Grading

	Weight
Homework	35% (7 total)
Tutorials	35% (6 total)
Final Projects	30%

VII Bibliography

Main Bibliography:

- F. de Groot, A. Kotani, Core Level Spectroscopy of Solids in: Advances in Condensed Matter Science, vol. 6, CRC Press, Boca Raton, FL, USA (2008), LC QC176.8.O6G76, 490 pp. (available electronically at the library)
- A.Frano Spin spirals and charge textures in transition-metal oxides heterostructures. Springer Thesis series (available electronically at the library)
- http://www.quanty.org

Complementary bibliography:

- J. van Bokhoven, C. Lamberti, X-ray absorption and X-ray emission spectroscopy : theory and applications, (available electronically at library)
- D.S. Rodgers, Circular dichroism: theory and spectroscopy
(available electronically at library).
- Philip Willmott, An Introduction to Synchrotron Radiation: Techniques and Applications
(available electronically at library).
- R.E. Peierls Quantum theory of solids, (General library - 530.41 P232)
- Mahan, G. D. (2000). Many-Particle Physics. Plenum Press.