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 BiFeO3 and rare earth nickelates RNiO3 (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

<table>
<thead>
<tr>
<th>Week</th>
<th>Topic</th>
<th>Quanty Tutorial</th>
<th>Homework</th>
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<tbody>
<tr>
<td>1</td>
<td>Introduction to core level spectroscopy</td>
<td>Tutorial #1: Quanty installation and first steps</td>
<td>-</td>
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<tr>
<td>2</td>
<td>X-Ray Fluorescence (XRF)</td>
<td>-</td>
<td>Homework #1: Introduction and XRF</td>
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<tr>
<td>3</td>
<td>Linear response theory</td>
<td>Tutorial #2: XRF Simulations, Basic spectrum simulation</td>
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<tr>
<td>4</td>
<td>Experimental tools</td>
<td>-</td>
<td>Homework #2: Linear response and Tools</td>
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<td>5</td>
<td>X-Ray Photoelectron Spectroscopy (XPS)</td>
<td>Tutorial #3: Simulations with different tools and devices, XPS Simulations</td>
<td>-</td>
</tr>
<tr>
<td>6</td>
<td>X-Ray Absorption Spectroscopy (XAS)</td>
<td>-</td>
<td>Homework #3: XPS and XAS</td>
</tr>
<tr>
<td>7</td>
<td>Electron-electron interactions</td>
<td>Tutorial #4: XAS Simulations, Modeling systems with strong interactions</td>
<td>-</td>
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### Week 8
- **Integrated Case Studies:** Batteries, Catalysts, Heterostructures and interfaces, Magnetic Materials
- **Homework #4:** Integrated case studies

### Week 9
- **Break - 30%**

### Week 10
- **Valence and core electron resonances**
- **Tutorial #5:** Resonance spectrum modeling

### Week 11
- **Spectroscopy in low dimensionality systems**
- **Homework #5:** Low dimensionality

### Week 12
- **Correlations and magnetism**
- **Tutorial #6:** Simulations in a selected correlated system (1D and 2D)

<table>
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<tr>
<th>Week</th>
<th>Topic</th>
<th>Quanty Tutorial</th>
<th>Homework</th>
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<tbody>
<tr>
<td>13</td>
<td>X-Ray Magnetic Circular Dichroism (XMCD) and related techniques</td>
<td>-</td>
<td>Homework #6: XMCD and applications</td>
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<tr>
<td>14</td>
<td>Disordered systems and liquids</td>
<td>-</td>
<td>Homework #7: Disordered systems and Advanced techniques</td>
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<tr>
<td>15</td>
<td>Advanced techniques in spectroscopy</td>
<td>Exploration of advanced features</td>
<td>-</td>
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<tr>
<td>16</td>
<td><strong>Review</strong></td>
<td>General review</td>
<td>Final Assessment</td>
</tr>
</tbody>
</table>

### 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:

- A.Franco 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)