

Resonant Inelastic X-ray Scattering: A Powerful Technique for Probing Materials

Resonant inelastic X-ray scattering (RIXS) is a powerful technique that combines spectroscopy and inelastic scattering to study the electronic structure of materials. It is based on the interaction of X-rays with matter, where RIXS spectra can be approximated as a combination of X-ray absorption and emission. RIXS allows for the investigation of collective excitations (magnons, phonons, plasmons, orbitons) in quantum materials and the exploration of material properties under operando or extreme conditions using hard X-rays. This article highlights recent advancements in RIXS instrumentation, data analysis, and applications. It also discusses the future of this spectroscopy with new experimental stations at free-electron lasers, which promise to revolutionize the study of ultrafast processes and nonlinear interactions of X-rays with matter.

RIXS is a chemically selective spectroscopy technique based on a two-step, two-photon resonant process. In RIXS, an incoming photon excites an electron, temporarily creating a hole in a core level. As the material returns to a lower energy state, it emits a photon with energy and wave vector different from the incident photon. The energy and momentum transferred to the system encode valuable information about it (see Fig. 1a). This two-step process enables the study of complex materials, revealing essential properties across diverse fields such as physics, chemistry, biology, and Earth sciences.

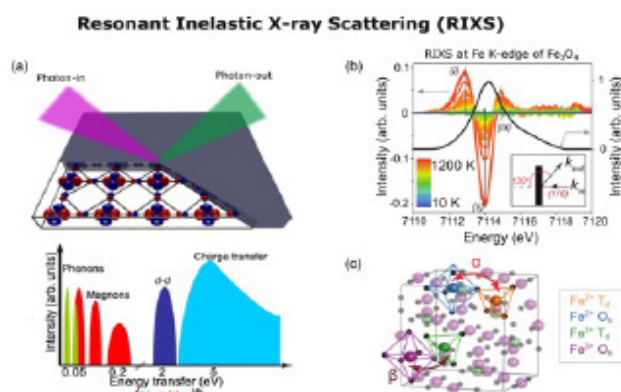


Figure 1

(a) Principle of RIXS spectroscopy. Various elementary excitations probed by RIXS in condensed matter and their associated energy scales. (b) High-energy resolved fluorescence detected Fe K α , a type of RIXS, measured in magnetite (Fe_3O_4) from 10 to 1200 K. Three peaks (i, ii, iii) are observed evolving with temperature. (c) Changes in the spectra are linked to charge transfer between octahedral and tetrahedral sites in magnetite [Elnaggar et al., *Phys. Rev. Lett.*, 127, 186402 (2021)].

In physics, RIXS has become a key tool for elucidating interactions in quantum materials. For example, high-temperature superconductors such as cuprates exhibit fascinating spin and charge dynamics that are challenging to analyse with traditional methods. RIXS can reveal the dispersion of collective excitations, such as magnons and charge density waves, shedding light on how spin and charge behaviour influences superconductivity and magnetism. This provides a basis for understanding exotic phases and guiding future applications. For instance, studies of charge order in magnetite (Fe_3O_4) across temperatures uncovered a previously unknown spontaneous charge order at high temperatures (see Fig. 1b-c).

RIXS also addresses complex questions in chemistry, particularly in catalysis and energy storage. By selectively probing catalyst elements, RIXS captures how oxidation states and electronic structures evolve under reaction conditions, identifying active sites and key reaction

mechanisms. Similarly, RIXS tracks structural changes in battery electrodes during charge and discharge cycles, offering critical insights into degradation processes and contributing to the design of more efficient and durable batteries.

In biology, RIXS effectively studies metal centres in proteins and enzymes, such as manganese in Photosystem II or iron in nitrogenase. Its chemical selectivity allows analysis of electronic configurations and oxidation states involved in redox and electron transfer processes, even in trace concentrations. These insights are essential for understanding fundamental biochemical mechanisms and may inform the design of biomimetic catalysts.

Finally, RIXS is highly valuable in Earth sciences, enabling the study of minerals and geochemical processes under extreme pressures and temperatures, such as those in Earth's core. RIXS reveals phase transitions in minerals and the behaviour of elements at depth, advancing our understanding of Earth's internal dynamics and the geochemical stability of elements in the mantle and core with unparalleled detail compared to conventional X-ray absorption or emission spectroscopy.

Though now a mature and interdisciplinary technique, RIXS holds exciting prospects with advanced experimental configurations and improved energy and momentum resolution. Enhancements in detector capabilities and overall count rates will facilitate new experiments, including RIXS microscopy. Dedicated reaction cells and sample environments will enable in situ or operando RIXS experiments. Additionally, the availability of RIXS beamlines at free-electron laser facilities opens new avenues, such as femtosecond time resolution and nonlinear phenomena exploration.

Reference

"Resonant inelastic X-ray scattering"

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