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Mapping Resonant Inelastic X-ray Scattering Onto Electronic Structure of Iridium Compounds

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ABSTRACT

Resonant inelastic X-ray scattering (RIXS) is an indispensable tool that can selectively probe the electronic structure of active sites in energy conversion systems, for example, iridium oxides. However, decoding the RIXS spectra remains challenging due to its inherently complex many-body interactions. Here, we analyze Ir L_3 edge RIXS spectra of Ir, IrCl₃, and IrO₂, employing the joint density of states (JDOS) calculated directly from electronic band-structure calculations. The overall energy-loss features in the RIXS spectra are well reproduced by the JDOS, reaffirming the close correspondence between electron–hole excitations and RIXS spectra observed in prior studies. Intriguingly, the RIXS spectra above ~ 4 eV in metallic Ir and IrO₂ follow a power-law behavior, $I_{\text{RIXS}} \propto \Delta^{-p}$, where Δ is the energy loss and p is the associated power-law exponent. This is consistent with edge-singularity behavior commonly found in resonant X-ray scattering from metallic samples. Furthermore, orbital-projected JDOS enables a decomposition of the IrO₂ spectrum into specific dd transitions, providing a clear interpretation of orbital excitations and an efficient strategy for decoding RIXS spectra in iridium-based energy conversion systems.

1 | Introduction

Resonant inelastic X-ray scattering (RIXS) serves as both an element-specific and bulk-sensitive spectroscopic tool for exploring orbital, charge, and magnetic excitations through resonant enhancement at the core-hole absorption edge. In material systems containing multiple atomic species, RIXS can selectively probe transitions associated with a specific element, thereby revealing direct insight into the electronic structure and underlying mechanisms. These RIXS signals encompass a wide range of intrinsic excitations, including orbital transitions, charge transfer, and magnetic transitions. Consequently, RIXS provides a powerful and uniquely informative approach for investigating the electronic structures of correlated electron systems and energy conversion materials, including iridium oxides that are both correlated 5d transition metal oxide systems and key materials in energy-conversion catalysis [1–10].

However, interpreting RIXS spectra remains challenging because of the inherently complex photon-matter interactions that govern the scattering process. The Kramers-Heisenberg formalism describes the RIXS process in which an incident photon excites a core electron into unoccupied states, creating intermediate states (X-ray absorption [XAS]). The subsequent radiative decay of this intermediate state into the final states yields the emitted photon (XES) [1, 2]. Because RIXS calculations must include intermediate and excited final states that deviate from the ground state, fully extracting quantitative information from the spectra becomes nontrivial. This challenge becomes even more significant for strongly correlated transition metal systems, as their many-body interactions require substantial computational resources in RIXS calculations [2, 7, 11–13].

Utilizing a ground-state approximation to the intermediate state in the Kramers-Heisenberg formalism, the RIXS process can be modeled as generating electron–hole excitations characterized by

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the joint density of states (JDOS). In this picture, RIXS simplifies to a convolution of XAS and X-ray emission (XES), which respectively examine the unoccupied and occupied electronic states [12, 13]. This framework naturally relates the RIXS spectra to the JDOS, as observed in optical transitions. Although previous studies have shown that JDOS-based descriptions can explain the specific characteristics of RIXS spectra in certain materials, the efficacy and feasibility of JDOS-based RIXS analysis for Ir 5d systems, especially in relation to energy conversion systems, remain inadequately examined, which requires more systematic investigation [1, 7, 14–17].

Here, we evaluate the capability of a JDOS framework to explain the RIXS spectra of three representative iridium compounds: the band insulator IrCl_3 , the band metal IrO_2 , and elemental Ir. Notably, despite the significant spin–orbit coupling and moderate correlation effects in these 5d systems, the JDOS reasonably reflects the main energy-loss features of the measured RIXS. This discovery highlights that the RIXS signal in iridium-based materials can be understood through an intuitive electron–hole excitation model, thereby establishing JDOS-based analysis as an effective and practical tool for decoding RIXS data in 5d transition-metal systems. Deviations observed in the metallic samples at higher energy losses (about 4 eV and above) indicate many-body effects aligned with the edge singularity effect, delineating the boundaries of the JDOS framework.

2 | Results and Discussion

Figure 1A and B shows the total Ir 5d density of states (DOS) of metallic Ir and insulating IrCl_3 compounds, obtained from Ref. [18] and the Materials Project database (version 2020_09_08), respectively [18–20]. As shown in Figure 1C and D, the Ir 5d JDOS results, denoted by red lines, were computed from the occupied and

unoccupied 5d DOS of both samples and represent the interband transitions between occupied and unoccupied states [21]. In our analysis, we use the total Ir 5d orbital projected DOS obtained from band-structure calculations of the compounds [18–20].

The JDOS is mathematically defined as

$$J(\Delta) = \int_E \rho_o(E) \rho_u(E + \Delta) dE \quad (1)$$

where ρ_o and ρ_u are occupied and unoccupied DOS, respectively. Based on a simplified treatment of the RIXS process [1, 7], the intensity can be approximately expressed as

$$I_{\text{RIXS}}(\omega_i, \Delta) \sim \int_E \frac{\rho_o(E) \rho_u(E + \omega)}{(E - \omega_i + \Delta)^2 + \Gamma^2/4} dE \quad (2)$$

where I_{RIXS} , Δ , ω_i , and Γ correspond to the RIXS intensity, energy loss, incident photon energy, and intermediate lifetime, respectively. Integrating this RIXS intensity over incident energies approximately yields the JDOS formula.

$$\begin{aligned} I_{\text{int}}(\Delta) &= \int_{\omega} I_{\text{RIXS}}(\omega, \Delta) d\omega \\ &\sim \int_{\omega} \int_E \frac{\rho_o(E) \rho_u(E + \omega)}{(E - \omega_i + \Delta)^2 + \Gamma^2/4} dE d\omega \\ &\sim \int_E \rho_o(E) \rho_u(E + \Delta) dE \end{aligned} \quad (3)$$

These results indicate that the incident-energy-integrated RIXS spectra in Figure 1C and D correlate with direct interband transitions between Ir 5d occupied and unoccupied states. Intriguingly, we found that the RIXS spectra up to ≈ 4 eV were

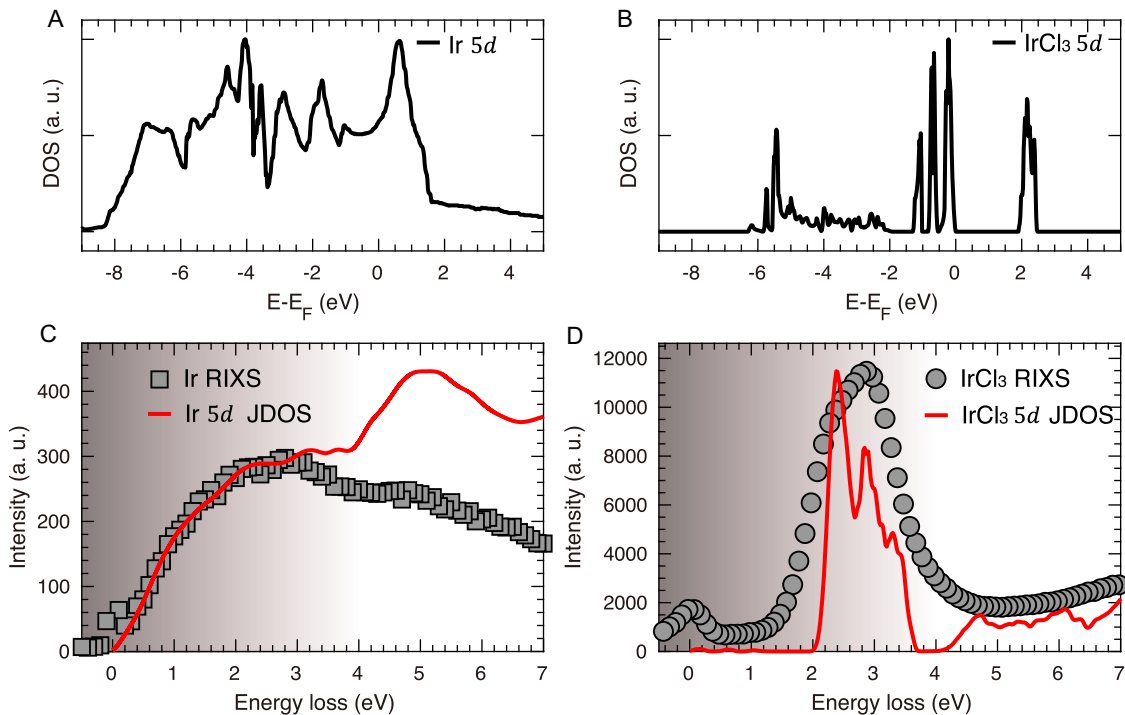


FIGURE 1 | Ir 5d density of states (DOS), JDOS and Ir L_3 edge RIXS spectra for Ir and IrCl_3 . (A) The Ir metal 5d DOS obtained from Ref. [18]. (B) The IrCl_3 insulator DOS was obtained from the Materials Project database (version 2020_09_08) [19, 20]. (C) Comparison of RIXS spectra with JDOS of Ir metal. (D) Comparison of IrCl_3 . Gray squares (Ir) and circles (IrCl_3) represents RIXS spectra. Integrating incident-energy-dependent RIXS spectra from 11.211 to 11.219 keV produces these RIXS spectra. The red line is the JDOS calculated from the Ir 5d DOS.

well captured by the JDOS calculations of the samples. In essence, the RIXS spectral feature in this energy-loss range predominantly arises from transitions between nearly unperturbed unoccupied and occupied states near the Fermi level.

There is a notable correspondence between the integrated RIXS spectra and the JDOS below an energy loss of ≈ 4 eV for both Ir metal and IrCl_3 insulator. As shown in Figure 1C and D, the brown-shaded loss features are quantitatively reproduced by the JDOS calculations. This energy range corresponds to the key chemical-bonding energy scale relevant to energy conversion processes [22]. In particular, the JDOS of the metallic system displayed in Figure 1C quantitatively matches the corresponding RIXS spectrum. In contrast, for the insulating IrCl_3 in Figure 1D,

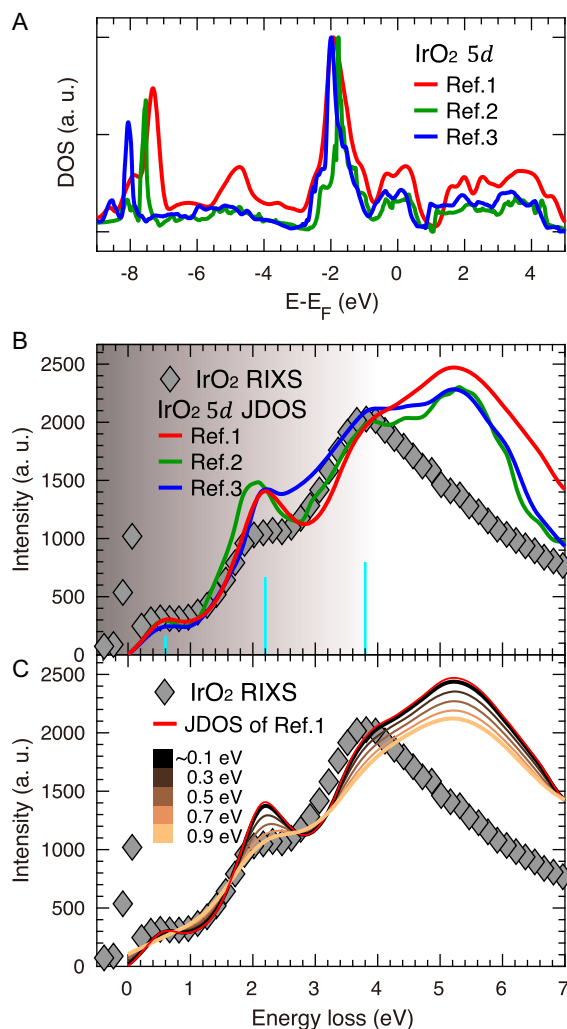


FIGURE 2 | JDOS results and Ir L_3 RIXS spectra for IrO_2 . (A) Ir 5d DOSs for rutile IrO_2 . The DOS results are extracted from the references denoted as Ref. 1 [8], Ref. 2 [19, 20] (from the Materials Project database (version 2020_09_08)), and Ref. 3 [23]. (B) Integrated RIXS spectrum and JDOS for rutile IrO_2 . The JDOS calculations are based on the DOS in (A). (C) Convolved JDOS results. The JDOS was convolved with a Pseudo-Voigt function whose parameters were determined by fitting the elastic peak in the integrated RIXS spectra (see Figure S1). Although the instrumental resolution is better than 0.1 eV, the FWHM was systematically varied from 0.1 to 0.9 eV to address the influence of additional broadening mechanisms, such as many-body effects and matrix-element effects.

the JDOS qualitatively reproduces the overall shape of the loss features across the entire energy range, extending even above 4 eV. Collectively, these findings highlight the need for a more comprehensive JDOS-based analysis of RIXS spectra in Ir 5d compounds.

To further verify the JDOS-based interpretation of Ir L_3 edge RIXS spectra, we also investigate rutile IrO_2 , which exhibits intermediate metallicity between Ir metal and IrCl_3 insulator, as shown in Figure 2. The Ir 5d DOS structure indicates that IrO_2 shows a bandwidth broader than that of IrCl_3 , yet more structured than that of metallic Ir, placing it electronically between these two extremes. IrO_2 has been extensively investigated as a model energy-conversion material, notably one of the most efficient catalysts for oxygen-evolution reaction in water splitting [8, 24]. Note that the Ir 5d orbital state in IrO_2 serves as a critical descriptor, which can govern its catalytic process [8, 25]. Consequently, systematic investigation of the Ir 5d orbital states in IrO_2 is essential using RIXS measurements.

Figure 2 shows the RIXS spectra of the IrO_2 metal oxide powder sample and the corresponding Ir 5d JDOS. This enables a direct comparison between the metallic (Ir) and insulating (IrCl_3) extremes. As shown in Figure 2A, DOS calculations of rutile IrO_2 were extracted from the references denoted as Ref. 1 [8], Ref. 2 [19, 20], and Ref. 3 [23]. Despite the variations in JDOS that result from multiple DFT results for rutile IrO_2 , all have corresponding peak positions at ≈ 0.6 , 2.2, and 3.8 eV. To evaluate the sensitivity of the JDOS in relation to band structure

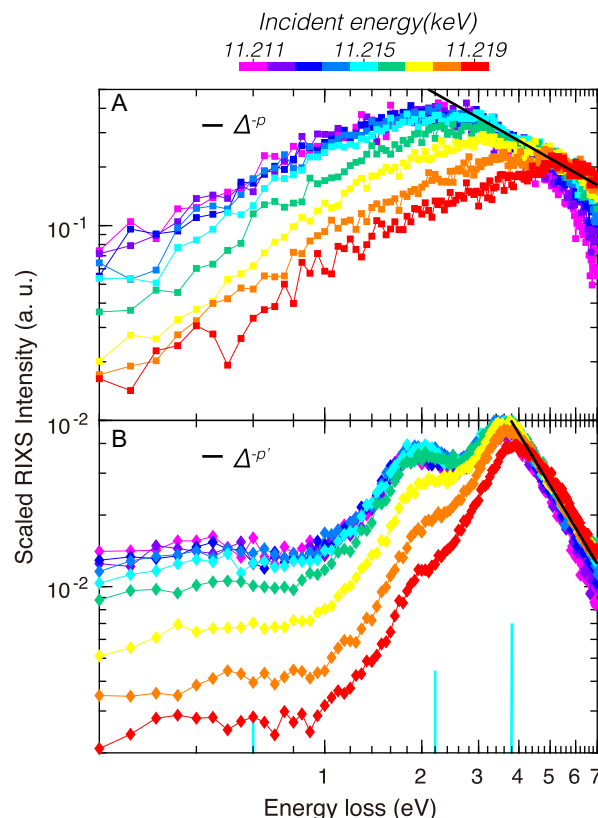


FIGURE 3 | (A,B) Scaled Ir L_3 edge RIXS spectra for Ir and IrO_2 . The incident energy-dependent RIXS spectra exhibit collapses at ≈ 4 eV energy loss. The tendency for this collapse can be assessed using power functions (Black solid lines) with constants, $p = 0.94$ (Ir) and 2.25 (IrO_2). The sky-blue bars represent energy loss positions of 0.6, 2.2, and 3.8 eV.

calculations for IrO_2 , we compute the JDOS using three band structure results. Remarkably, the three JDOS representations have consistent main peak features, as indicated by the sky-blue bar in Figure 2B. Although the spectral weight of peak features in the RIXS spectrum below 4 eV diverges from the JDOS results, the JDOS closely aligns with the RIXS spectrum in this energy range, based on direct calculations that exclude the transition matrix and spectral function [1, 12, 13].

As shown in Figure 2C, we investigate the effect of instrumental energy resolution on the JDOS by explicitly modeling the spectral broadening. The instrumental resolution of the IrO_2 RIXS spectrum was independently determined to be ≈ 90 meV (a full width at half maximum, FWHM) from elastic peak fitting, as shown in Figure S1. Using the resolution of 0.1 eV, the JDOS was convoluted with a Pseudo-Voigt function, characterized by 65% contribution ratio of Gaussian and Lorentzian components, to generate a broadened spectral line shape (Figure 2C and Figure S2) [26–28].

Furthermore, to evaluate the sensitivity of the JDOS-RIXS comparison to instrumental broadening, the FWHM was systematically varied from 0.1 to 0.9 eV (Figure 2C). In the low-energy region, the agreement between the broadened JDOS and the RIXS spectra requires broadening significantly exceeding the instrumental resolution, pointing to intrinsic contributions beyond instrumental

effects. At higher energy losses above around 4 eV, the JDOS systematically overestimates the RIXS spectral weight even when substantially larger broadening is applied. The discrepancy therefore reflects matrix-element effects and many-body contributions in metallic IrO_2 beyond the JDOS approximation. The details of the RIXS process and momentum-dependent JDOS (Figure S3) were described in Supplementary Information Part 2.

Figure 3 shows that in metallic iridium compounds, such as Ir in Figure 3A and IrO_2 in B, RIXS spectra at various incident energies ranging from 11.211 to 11.219 keV display a power-law decay characteristic above ≈ 4 eV. Building upon the previous analysis, we observe comparable discrepancies between the JDOS and RIXS spectra above ≈ 4 eV in these two metallic iridium-based samples. Specifically, beyond 4 eV, the integrated RIXS spectra demonstrate a decaying trend, whereas the JDOS exhibits more pronounced peak structures. This discrepancy between the JDOS and RIXS spectra above 4 eV might stem from a reduction in direct interband transitions (i.e., dipole transitions) and an increase in multiple interaction in this energy range. To investigate this decaying feature, we fit incident energy-dependent RIXS spectra with a power function for each sample. We tried to interpret this phenomenon as the edge singularity effect observed in resonant experiments conducted on metallic samples [29, 30].

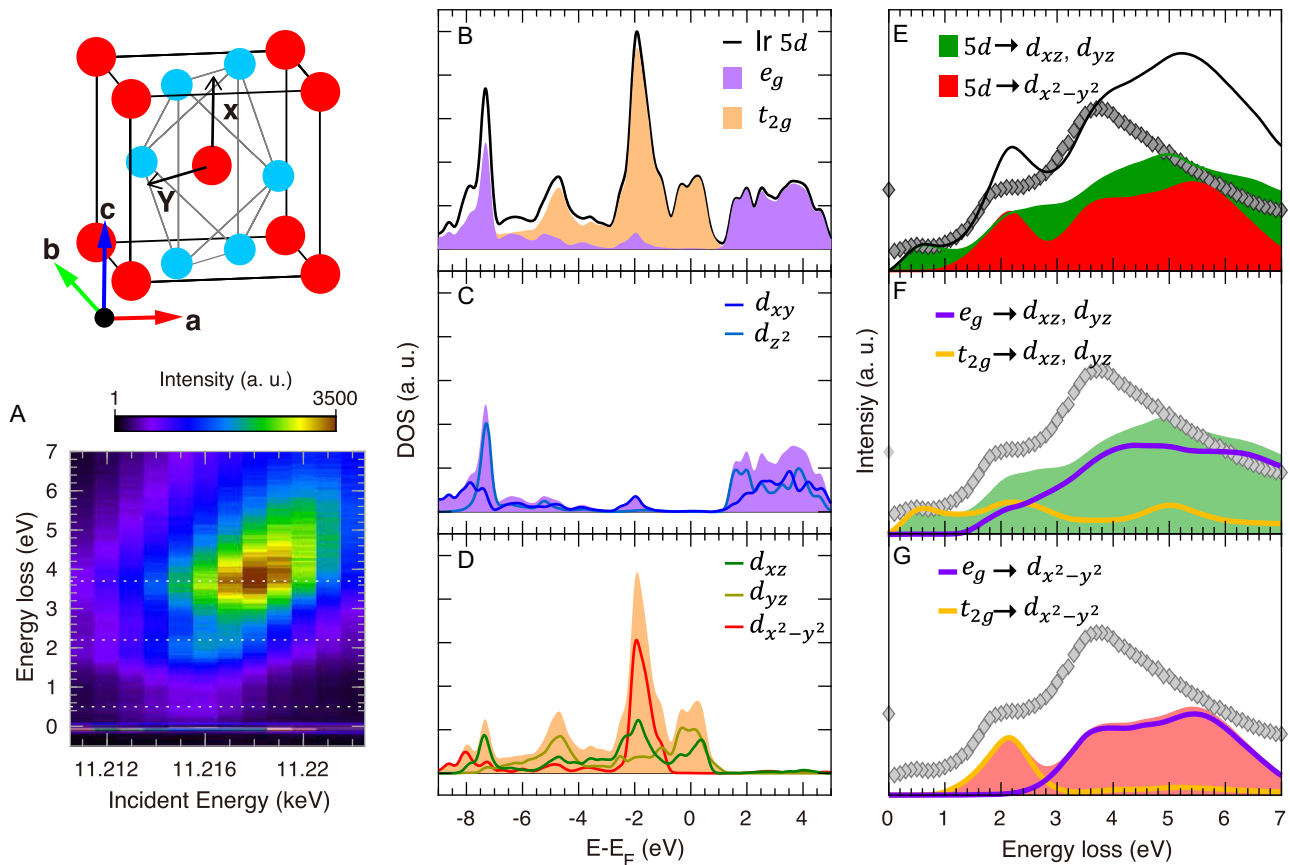


FIGURE 4 | Orbital-projected JDOS for rutile IrO_2 . (A) Incident energy dependence of RIXS mapping with the structure of rutile IrO_2 . (B–D) Ir 5d total DOS (B) and the projected DOS (pDOS) results for rutile IrO_2 obtained from the reference [8]. Colored lines show the pDOS of (C) e_g and (D) t_{2g} orbitals, defined as the x, y, z orientation [34]. (E–G) Orbital projected JDOS and RIXS spectra, calculated from the pDOS results represented in B–D. The green color in E and F represents transitions between unoccupied Ir 5d DOS and occupied d_{xz} and d_{yz} pDOS. The red color in E and G represents transitions between unoccupied Ir 5d DOS and occupied $d_{x^2-y^2}$ pDOS. The purple and orange colors in F and G represent the partial JDOS results obtained from unoccupied e_g and unoccupied t_{2g} pDOS, respectively.

This power-law behavior could be elucidated in terms of an edge-singularity-type process, originating from the scattering between the core-hole potential and electrons near the Fermi level in the intermediate state of the RIXS process. Such scattering events induce a phase shift in the electronic wave functions, which determines the power-law exponent. Qualitatively, a higher DOS near the Fermi level reduces the phase shift and leads to a reduced exponent. Consequently, the lower exponent observed in Ir metal indicates a higher DOS near the Fermi level compared to IrO₂ [30–32].

Note that the threshold can be empirically estimated as the characteristic energy scale below which one electron-hole pair and excitonic excitations predominantly evolve. The main peak features (marked as sky-blue bar in Figure 3B) in IrO₂ RIXS spectra exhibit a linear Raman dispersion feature [33], maintaining a constant energy difference relative to incident energy. These peaks are observed below the threshold energy of 4 eV. In the case of Ir metal, the main peak, about 2 eV, corresponds with the Raman feature, that is, below the resonant incident energy of 11.215 k eV, this peak pattern remains consistent up to the threshold. Furthermore, following the resonant incident energy, the fluorescent signals with a constant emission energy of about 11.215 k eV emerge. These fluorescence promptly follow the power-law decaying after peak positions, as these peak positions exceed the threshold. This finding indicates that the threshold is reasonable for assigning the characteristic energy scale for excitonic feature [13, 29, 30].

We deconvolute both DOS and JDOS based on orbital-projected DOS (pDOS) to examine the elementary excitations of IrO₂, including dd transitions, as shown in Figure 4. Figure 4A displays the incident energy-dependent RIXS mapping of rutile IrO₂, exhibiting distinct peak features at ≈ 0.6 , 2.2, and 3.8 eV, shown by the white dashed lines. Note that excitonic characteristics can originate from electron-hole pairs in the 5d orbital states. Figure 4B illustrates the total DOS of Ir 5d, which has been deconvoluted into the e_g (Figure 4C) and t_{2g} orbitals (Figure 4D).

Because the IrO₆ octahedra in rutile IrO₂ are edge-sharing (Figure 4A), the t_{2g} states are most naturally classified by spatial orientation (Figure 4C), and the hole component of the excitation resides within one of these orbitals. For instance, $d_{x^2-y^2}$ is located at the octahedra-edge-sharing plane, whereas the other group includes d_{xz} and d_{yz} , which lie perpendicular to the plane [34, 35]. Based on these JDOS calculations (Figure 4E), the pronounced peak feature observed at ≈ 2.2 eV is attributed to the hole in $d_{x^2-y^2}$ orbital, as shown in Figure 4F and G. Furthermore, the ≈ 0.6 eV peak feature is dominantly generated by the hole in d_{xz} and d_{yz} orbitals (Figure 4F). The geometric classification captures the Ir-O hybridization characteristic of rutile IrO₂.

Within the JDOS-based framework and the edge singularity effect, the overall RIXS spectra can be understood and analyzed through the hole and electron components of electron-hole pairs in IrO₂. Specifically, when the hole states of electron-hole pair in RIXS process correspond to d_{xz} and d_{yz} , the electron state of electron-hole pair within t_{2g} the orbitals predominantly determines the profile of the JDOS below 1 eV and exhibits a constant spectral contribution across the entire JDOS as shown in Figure 4F. Notably, the electron state of electron-hole pair in t_{2g} not only contributes to all of the low-energy transitions below about 1 eV but also a substantial influence on the features of the peak around

2.2 eV. In contrast, the ≈ 3.8 eV peak feature is strongly related to the electron state of electron-hole pairs in e_g orbitals. As the energy scale of the peak increases, a larger number of Ir 5d orbitals becomes correlated. The spectral intensities of high-energy features over 4 eV are significantly dampened in the experimental spectra, suggesting that electron-hole pairing is ineffective beyond this threshold. Overall, this reflects the broader hybridization and multiple scattering of interband transitions in iridium-based materials.

3 | Conclusion

We report a comparison of RIXS spectra with the electronic band structures of iridium compounds. The band insulator IrCl₃, the band metal IrO₂, and Ir-metal powders are examined due to their technological importance and well-defined electronic band structures. RIXS spectra were collected across the Ir L₃-edge absorption, and integrated spectra were obtained by summing up over all incident photon energies to capture all excitations. The JDOS is a good representation of electron-hole excitations and is calculated from electronic band structure calculations. We find that excitation features are in excellent agreement with the experimental spectra and the JDOS. This work supports a direct comparison between RIXS spectra and JDOS derived from electronic band structures of band insulator and metal Ir compounds. This provides an efficient method to achieve a microscopic understanding of the electronic band structures of technologically significant Ir compounds.

4 | Experimental Section

IrCl₃ (Sigma-Aldrich : 520 721), IrO₂ (Sigma-Aldrich : 206 237), and Ir-metal (Sigma-Aldrich : 209 688) were used in this study. The RIXS measurements were conducted using the spectrometer at the 27-ID beamline at the Advanced Photon Source. X-rays were monochromatized to a bandwidth of 70 meV. The incident X-ray is focused to 50 (horizontal) X 20 (vertical) μm^2 . A horizontal scattering geometry was used with the incident photon polarization in the scattering plane to minimize the elastic scattering. For the L₃-edge RIXS, a Si(844) diced spherical analyzer with 4-inch radius and a position-sensitive silicon microstrip detector were used in the 1 m Rowland geometry. The overall energy resolution of the RIXS spectrometer at both edge was 100 meV, as determined from the full-width-half-maximum (FWHM) of the elastic peak.

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Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Supporting Information

Additional supporting information can be found online in the Supporting Information section. **Supporting Fig. S1:** Results of elastic peak fitting. **A–C** Fitting of the elastic signal in the integrated RIXS spectra for (A) Ir, (B) IrO₂ and (C) IrCl₃. **Supporting Fig.S2:** Effect of instrumental broadening on the joint density of states (JDOS). **A** Fitting of the elastic noise signal in the IrO₂ powder RIXS spectrum. A pseudo-Voigt fit yields an instrumental resolution (FWHM) of approximately 90 meV and a Gaussian contribution that amounts to 65%. **B** Comparison among the experimental RIXS spectrum (square), JDOS computed from the DOS in Ref. S[1] (blue line), and broadened (convoluted) JDOS incorporating the instrumental resolution of 90 meV (red line). **Supporting Fig. S3:** Momentum-dependent JDOS analysis. **A** Momentum dependent Ir 5d partial density of states (DOS) adapted from Ref. S[4]. **B** The corresponding momentum-dependent JDOS spectra. Each JDOS curve is derived from the specific momentum-projected DOS shown in **A**. **Supporting Table S1:** Pseudo-Voigt fitting parameters for the elastic signal.