Vibronic excitations in the resonant inelastic x-ray scattering spectra of spin-orbit Mott insulators

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Resonant inelastic x-ray scattering (RIXS) spectroscopy is a powerful tool to investigate elementary excitations in spin-orbit Mott insulators. Recent RIXS data of cubic Ru^{4+} and Ir^{4+} antifluorites (K_2RuCl_6, K_2IrCl_6, K_2IrBr_6) show puzzling features that cannot be explained by spin-orbit theories. As the origin of the features, the dynamic Jahn-Teller effect was considered as a possible scenario [1,2], whereas the evidence and its fingerprints in the RIXS spectra are unknown. Here, we address these issues based on *ab initio* calculations [3]. We simulated the RIXS spectra fully taking account of the dynamic Jahn-Teller effect, which shows a good agreement with the experimental spectra, confirming the presence of the dynamic Jahn-Teller effect in the excited states of the 4d and 5d spin-orbit Mott insulators. We revealed that the experimental RIXS spectra have several peaks that come from the dynamic Jahn-Teller effect rather than the standard crystal-field splitting. Our results suggest that the dynamic Jahn-Teller effect is an important factor in adequately interpreting the RIXS spectra of spin-orbit Mott insulators.

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