Vibronic effects in resonant inelastic x-ray scattering of a cubic 5d^1 Rhenium oxide

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We applied the equation-of-motion coupled cluster (EOM-CC) method to the derivation of the dynamic Jahn-Teller (JT) model for the 5d^1 Re centers in Ba_2MgReO_6. The derived interaction parameters are found to be close to those extracted from the experimental Re L_3 edge resonant inelastic x-ray scattering (RIXS) spectra [1]. In particular, the EOM-CC method also allowed for determining the weak vibronic coupling to the T_{2g} vibrations, which is difficult to address experimentally.

With the derived dynamic JT model for the Re centers, we calculated the corresponding local vibronic states and, on this basis, simulated the Re L_3 edge RIXS spectra (Figure 1). The simulated spectra indicate that vibronic coupling to the T_{2g} modes gives rise to a shoulder on the elastic peak, whose origin has previously been unclear [1].

The present simulations suggest that the dynamic JT effect involving both the E_g and T_{2g} modes is indispensable for a decent description of the multipolar phenomena in the investigated compound. This work also demonstrates that the EOM-CC method is a powerful tool for accurately predicting the complex local states at metal sites in correlated insulating materials.
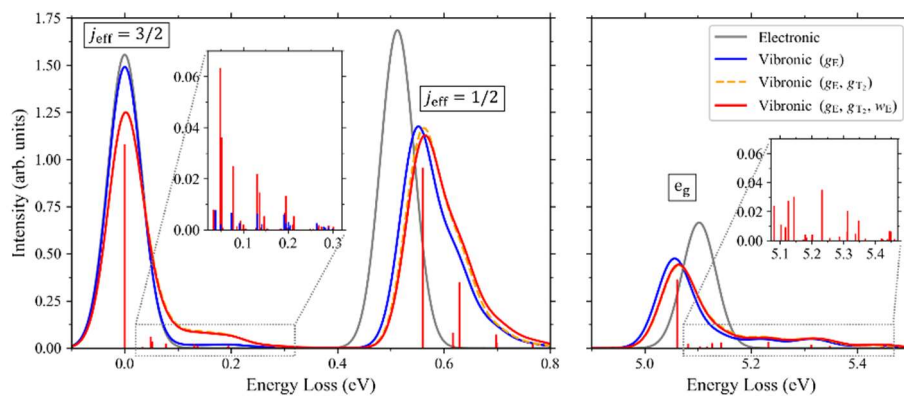
Figure 1. Simulated Re L_3 edge RIXS spectra.

Reference

[1] F. I. Frontini *et al*., Phys. Rev. Lett. **133**, 036501 (2024).