Electron Hole Excitations in Transition Metals Investigated via Inelastic X-ray Scattering: A Theoretical Perspective

A. G. Eguiluz,[1,2] I. G. de Gurtubay,[3] W. Ku,[4] B. C. Larson,[2] J. Z. Tischler,[2] P. Zschack[5]
[1]University of Tennessee, Oak Ridge, TN, U.S.A.
[2]Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, U.S.A.
[3]University of the Basque Country, Spain
[4]University of California, Davis, CA, U.S.A.
[5]University-National Laboratory-Industry Collaborative Access Team (UNI-CAT) and
Materials Research Laboratory (MRL), University of Illinois at Urbana-Champaign (UIUC), Urbana, IL, U.S.A.

Introduction

Inelastic x-ray scattering (IXS) is an ideal probe of the electron-hole excitation "channels" in condensed matter. Our ongoing research program, which builds on the power of a new breed of *ab initio*, all-electron, time-dependent density-functional theory (TDDFT) methods [1], is designed to produce fundamental new insight into the physics of correlated materials, starting from the nontrivial transition metals and their oxides. Still, because the correlation problem in these materials does not benefit from the existence of a "small parameter," the theoretical insight must rely strongly on the feedback provided by experiments performed at third-generation sources such as the APS.

Methods, Materials, and Results

Figure 1 displays representative results for Cr metal. We stress that the theoretical and the measured loss spectra (circles) are in absolute units. Thin solid lines refer to the random-phase approximation, which ignores the electron-hole interactions; thick solid lines refer to the time-dependent local density approximation (TDLDA), which invokes a simplified treatment of the "many-body kernel," involving the use of an adiabatic approximation, and the neglect of effects beyond the LDA. Clearly, the TDLDA does quite well — a success that could not have been predicted. Most importantly, the spectra show the emergence of a sharp peak at ~4 eV. Preliminary analysis suggests that this peak is a result of *d*-to-*d* transitions, involving narrow *d* complexes lying below and above the Fermi surface [2]. This electron-hole excitation, which is forbidden for small wave vectors, illustrates in a striking fashion the new capabilities of IXS for the investigation of electronic structure in correlated materials.

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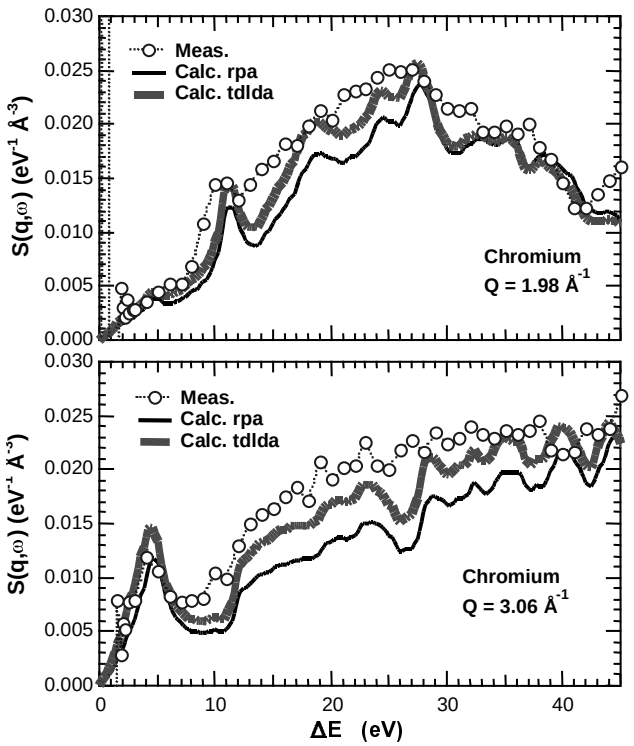

FIG. 1. TDDFT calculations and IXS measurements of the dynamical-structure factor S(q,ω) of Cr for two wavelengths.

References

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