ESRF	**Experiment title:** Dynamic structure factor of cuprate superconductors	**Experiment number:** HE-2143
Beamline: ID16	**Date of experiment:** from: 16-Mar-2006 to: 22-Mar-2006	**Date of report:** 1-Sep-2006(v1) 1-Sep-2010(v2)
Shifts: 18	**Local contact(s):** Dr. Gy. Vankó	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):
S. Huotari*, G. Monaco*, Gy. Vanko*
ESRF

Report:
The experiment to measure the dynamic structure factor in the plasmon limit of a sample of $YBa_2Cu_3O_{6.93}$ was performed at the beamline ID16. The purpose of the experiment was twofold: a) to study the valence excitations and the $S(\mathbf{q},\omega)$ in this strongly correlated high-T_C material as a function of momentum (q) and energy (ω) transfer; and b) to study the usefulness of non-resonant IXS in the study of high-T_C superconductors, a task never tried before to the authors' knowledge, the reason being the relatively low count rates achievable in non-resonant IXS from high-Z materials.

The results of this experiment have been published in S. Huotari, J. A. Soininen, G. Vankó, G. Monaco, and V. Olevano, Phys. Rev. B 82, 064514 (2010). Most important results are reproduced on page 2 of this report.

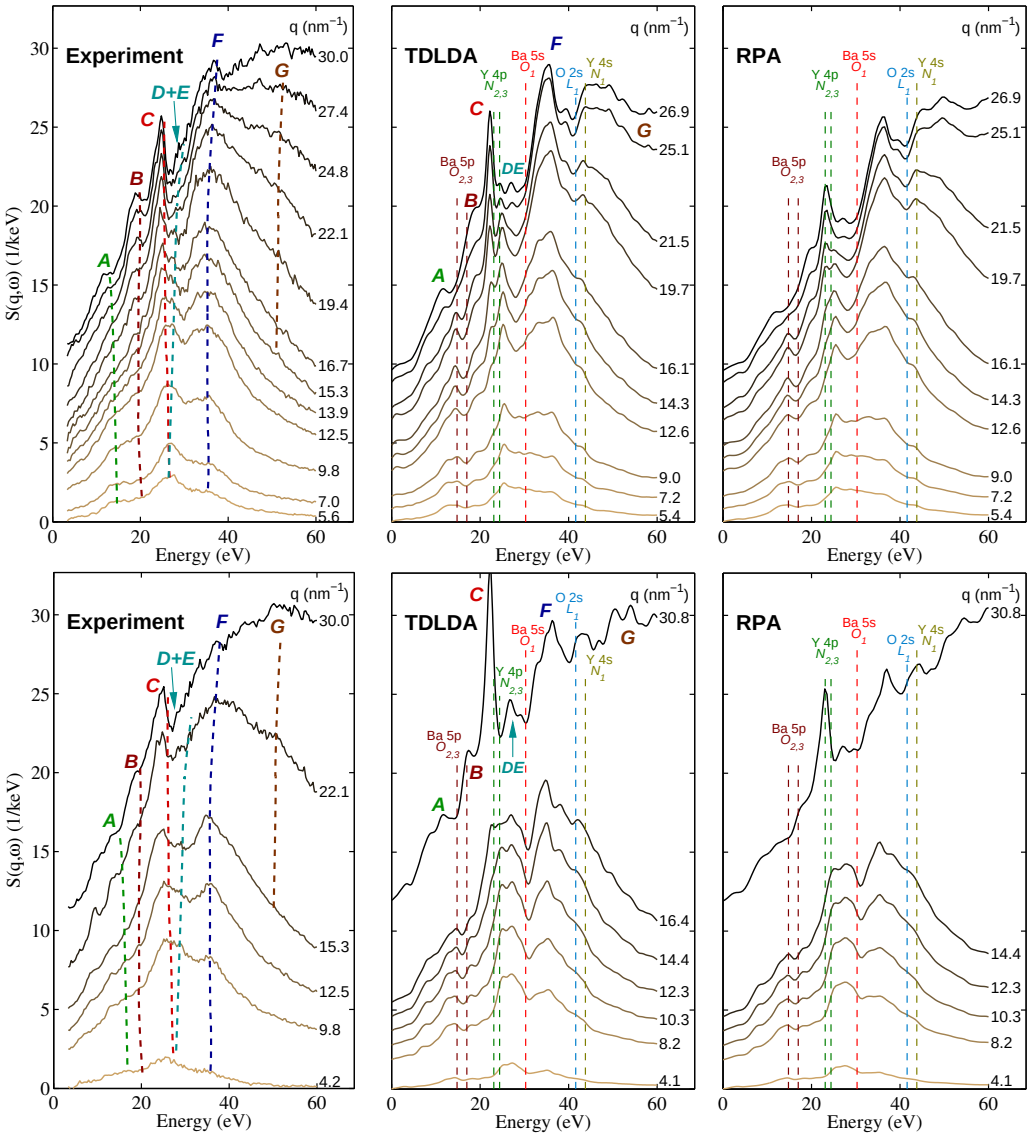

Figure 1

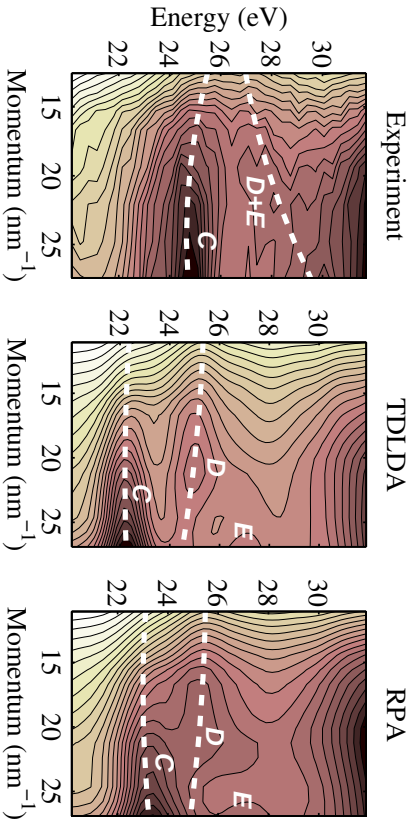

Figure 2

Figure 1. Experimental and calculated energy-loss functions of YBCO for **q** || **c** (upper panels) and **q** ⊥ **c** (lower panels). The most prominent spectral features are marked A–G and highlighed with dashed lines in the experimental plots. The nominal core-electron excitation energies are marked with dashed lines and labeled accordingly in the theory plots. It is astonishing how well an *ab initio* theoretical treatments within the TDDFT can reproduce the extremely finely structured experimental result – very few earlier result can compare with the perfect agreement, especially considering the level of sophistication of the theory. (From Ref. [1])

Figure 2. Zoom-up to the region of 20–32 eV energy transfer to show dispersing excitations C–E. It is in this region where the difference between TDDFT and the experiment is the most pronounced. In RPA the peaks D and E are broad and weak, but appear better defined in TDLDA. On the other hand, experimentally there are only two excitations, labeled tentatively as C and D+E. The peaks are reproduced by the theory but a discrepancy between the experiment remains. This could be one of the key differences where a treatment of correlations beyond TDLDA is necessary. (From Ref. [1]).

[1] S. Huotari et al. *Screening in $YBa_2Cu_3O_{7-\delta}$ at large wave vectors*, Phys. Rev. B 82, 064514 (2010)