ESRF	**Experiment title:** Momentum Dependence of Fluorine K-edge Core Exciton in LiF	**Experiment number:** HE-792
Beamline: ID16	**Date of experiment:** from: 7 April 2000 to: 14 April 2000	**Date of report:** 1 March 2000
Shifts: 15	**Local contact(s):** A. Shukla, J.P. Rueff	*Received at ESRF:*

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Report:

We have measured the non-resonant inelastic x-ray scattering spectra of lithium fluoride with an energy loss close to the fluorine K-edge. The momentum dependence of the spectra has been studied using several momentum transfer values and clear deviations from the dipole approximation are observed. Our theoretical approach uses a recently developed *ab initio* computational scheme, which takes properly into account the electron-hole interaction. A similar method has been succesfully used to study valence excitations in diamond and LiF [1]. Using this scheme, we show, that the observed deviations are due to an s-type exciton.

Energy transfer scans were performed in the inverse-energy scan geometry, i.e. the scattered energy was kept fixed, while the incident energy was tuned. Scattered energies of 9.911 keV and 7.922 keV were used, which were dictated by the analyser crystal. A single crystal LiF sample was used, having dimensions of 25 mm $\times$ 10 mm $\times$ 0.4 mm. Both transmission and reflection geometries were employed in the experiment. The momentum transfer was kept fixed along the (100) direction of the conventional cubic unit cell of LiF.

Our main results are shown in to following two figures. The inelastic scattering spectra over a wide energy loss range is shown in **Figure 1** using several momentum transfer values.

Clearly, the agreement between the experimental and theoretical data is remarkable over the whole energy- and momentum transfer ranges. The experimental data is scaled by a constant, in order to give the same integrated intensity over the measured energy range, which can be justified by the sum rules.

The near-edge region of the fluorine K-edge is shown in **Figure 2**. Both experimental and theoretical spectra are normalised to have the same area under the curves for energies above 693.5 eV, which was done to emphasize the momentum transfer dependence of different structures. According to other experimental [2] and calculated [3] absorption spectra, the features over 693.5 eV can be attributed to dipole allowed transitions. We, however, observe a peak below the edge with a momentum transfer dependence of its intensity, that differs from the dipole transitions. Using our calculations, we can conclude that the peak is due to an s-type core exciton.

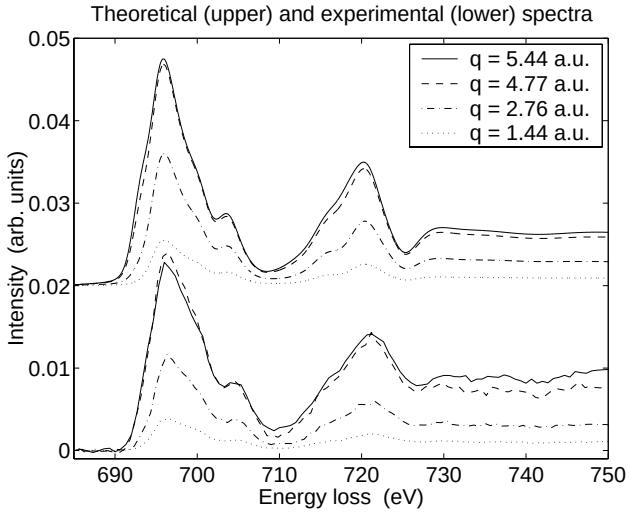

Figure 1

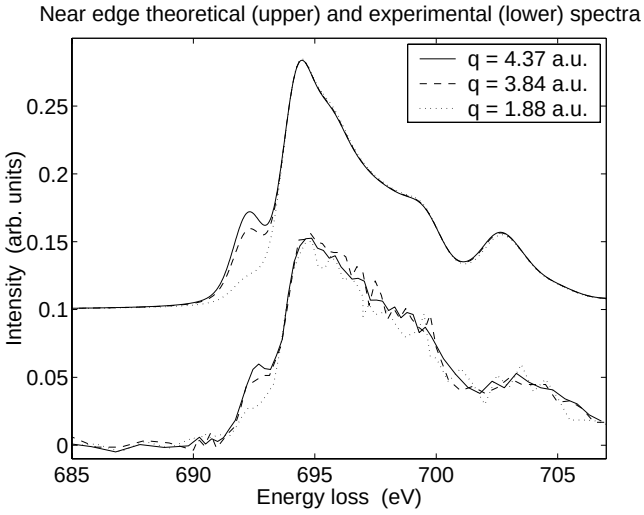

Figure 2

References

[1] W. A. Caliebe, J. A. Soininen, E. L. Shirley, C.-C. Kao, K. Hämäläinen, Phys. Rev. Lett. **84**, 3907 (2000)

[2] E. Hudson, E. Moler, Y. Zheng, S. Kellar, P. Heimann, Z. Hussain, and D. A. Shirley, Phys. Rev. B **49**, 3701 (1994).

[3] J.A. Soininen and E.L. Shirley, Submitted to PRB.