

A C K-edge X-ray Emission and Absorption Study of the Organic Semiconductor 8-Hydroxyquinoline Aluminum (Alq₃)

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Beamline(s): X1B

Introduction: The field of organic LED display technology and organic based electronics in general is currently an area of intense research. It promises the development of efficient, cheap, bright, thin and flexible displays that are expected to replace LCD type displays in many applications. The electro-luminescent organic compound 8-hydroxyquinoline aluminum (Alq₃) has proven to be quite useful in the construction of these devices due to its high fluorescence efficiency and the ease with which thin films may be deposited by thermal evaporation in vacuum. Naturally a solid understanding of the electronic structure of this material both in the bulk and at interfaces with metals or other organic materials is important if the performance of these devices is to be optimized. To this end we present a preliminary study of the carbon 2p partial density of states of Alq₃ as measured by the techniques of soft x-ray emission and absorption spectroscopy.

Methods and Materials: A Nordgren-type high resolution, grazing incidence, soft x-ray spectrometer was used to acquire the XES data presented here. The resolution of both the incident photon beam and x-ray spectrometer was 0.4eV. The XAS spectra were measured in total fluorescence yield mode via a large area x-ray diode positioned above the sample. XAS spectra were taken with a resolution of 0.1eV. The Alq₃ used in this study was in the form of a thin amorphous film (1um) that was deposited by thermal evaporation in vacuum onto a freshly cleaved KBr substrate. The film was subsequently transferred under vacuum into the UHV measurement chamber. Alq₃ like many organic compounds, is subject to changes in structure due to beam induced damage and steps must be taken to remove any of these effects from the data. This was achieved by utilizing a small beam size (50um) and continuously translating the film in front of the fixed synchrotron beam and spectrometer. This effectively exposes each section of the sample to only 2 seconds of light compared to the 30 minutes required to measure a typical XES spectrum.

Results: Presented in fig. 1a is a series of Alq₃ XES spectra acquired with incident photon energies near the carbon K-edge and a moving sample. The excitation energies are indicated on the XAS spectrum in fig.1b. The broad central feature is the carbon 2p PDOS, with a shape characteristic of molecules containing conjugated carbon bonds. Changes in the XES spectrum above threshold can be attributed to the progressive excitation of several slightly different C 1s core hole states at the chemically nonequivalent carbon sites. The strong feature to the right is produced by elastically scattered synchrotron light. Both XES spectra presented in fig. 2 were taken with an incident photon energy of 284.35eV but during acquisition of the blue spectrum the sample was moving while for the red it was fixed. The degradation of spectral features by beam damage is particularly evident for the HOMO state at the top of the valence band (280.5eV). A UPS spectrum from [1] is also plotted to indicate the correspondence between the states observed by XES and UPS.

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References: [1] H. Ishii et al. "Electronic Structure of 8-Hydroxy..." *Synthetic Metals*, **85**, (1997), 1389-1390

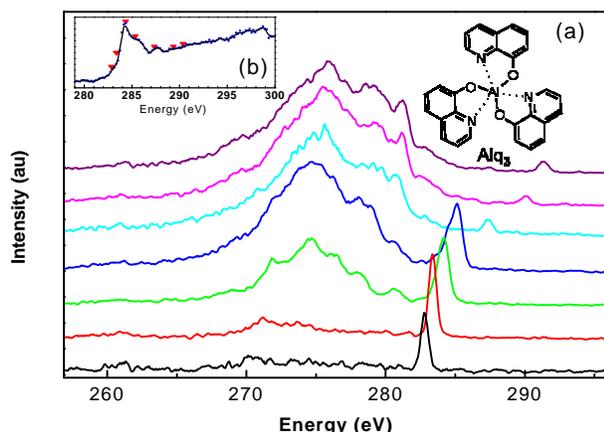


Figure 1. (a). C K-edge XES spectra measured with incident photon energies as indicated in the XAS spectrum (b).

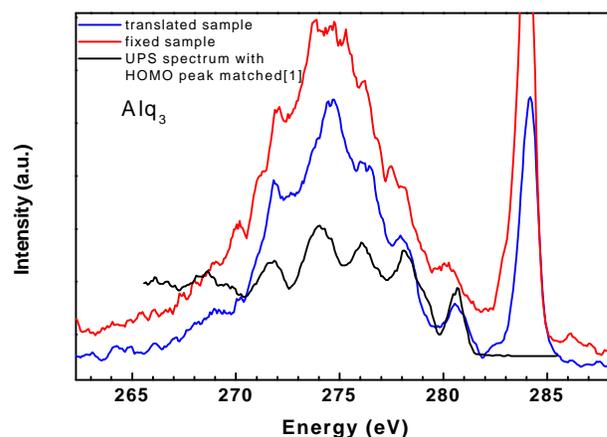


Figure 2. Comparison of fixed vs. moving sample spectra with the UPS spectrum from [1] superimposed.