Momentum Dependence of $\pi-\pi^*$ Excitations of Benzene Rings in Condensed Phases
H. Hayashi, N. Watanabe, Y. Udagawa (Tohoku U.), and C.-C. Kao (NSLS)
Abstract No. Haya1243
Beamline(s): X21

Introduction: The measurements of the real ($\varepsilon_1$) and the imaginary ($\varepsilon_2$) parts of the dielectric function (DF) over a complete momentum ($q$) - energy ($E$) range provide a crucial basis for studies of radiation in matter. Unfortunately, knowledge of the DF for molecular liquids is quite insufficient, especially for $q \sim 1$, because of the lack of appropriate experimental tools. With the developments of synchrotron radiation sources, however, it is now possible to apply inelastic x-ray scattering (IXS) to determine the DF of molecular liquids for $q \ll 1$.

Methods and Materials: IXS spectra for the $\pi-\pi^*$ excitation of liquid benzene have been measured for $0.35<q<1.5\text{Å}^{-1}$ at the X21, with 0.5eV-resolution for $E<10\text{eV}$ to resolve the $\pi-\pi^*$ peak and 1.3eV-resolution for $E>10\text{eV}$ to achieve high S/N ratio.

Results: The $\varepsilon_1$ and the $\varepsilon_2$ of benzene were deduced from the IXS spectra via the Kramers-Kronig transformation, and were shown in Fig. 1. Although the $\pi-\pi^*$ peak in the IXS profiles shows a negative $q$-dispersion (~0.5eV), no marked peak dispersion is found for the $\varepsilon_2$, indicating that the $\pi-\pi^*$ excitation in liquid is well localized. On the other hand, the amplitude of the variation in the $\varepsilon_1$ is reduced significantly as $q$ increases. Thus the negative dispersion in the IXS spectra must be attributed to changes of the shielding factor, $\varepsilon_1^{-2}+\varepsilon_2^{-2}$. This result means that the experimental deduction of not only energy-loss spectra but also DF on target molecular condensates is indispensable.