Inelastic X-ray Scattering of Molecules in Gas Phase

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Inelastic x-ray scattering (IXS) has proven to be a powerful tool for investigating the electronic excitations in inorganic systems [1]. In our previous work, we have successfully utilized the inelastic x-ray scattering (IXS) technique to study the exciton properties in small organic molecule crystal (Py-SO) at BL12XU of SPring-8 [2] and tried this technique on other complex organic crystals, including C60 single crystal, TTF-TCNQ, TEA-TCNQ and well oriented nano-tubes. The experiment results are very clean and therefore can be directly compared with theory. Our previous work proves that the modern non-resonant IXS is feasible for studying electronic excitation of organic molecular crystal. In this report, we extend this technique to the study of the excitations of gas phase molecules including monatomic molecule of Helium and diatomic molecules of Nitrogen and Hydrogen.

For the IXS experiment of gas phase Helium, the gas pressure of Helium is 3 atm. As we known, the uniqueness of the IXS is it provides the q resolution of the excitation. This can be used to study dipole forbidden transitions at high q region where dipole approximate broken is an important merit of IXS, which is unavailable for conventional optical techniques. For Helium, we observed very clearly monopole transition (1s-2s). The intensity of monopole transition is even stronger than dipole transition at high q which is unexpected.

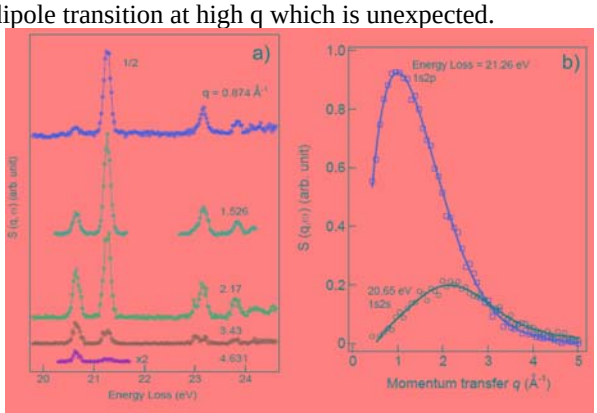

Figure 01 IXS spectra of Helium

Fig 1a. shows the IXS spectra of Helium. The q range is from 0.874 to 4.631. On the spectra the monopole transition and dipole transition are clearly observed. Monopole transition (1s-2s) energy is at 20.65eV, dipole (1s-2p) is at 21.26eV. Higher energy features involve many different transitions. Fig 1b. indicates the q dependences of the peak intensity for 1s-2s and 1s-2p. The intensity of monopole is even stronger when q is larger than 3Å-1. This is a very interesting phenomenon. We are collaborating with theorist for further calculation.

We also studied the electronic structure of the excited states of the gas phase Hydrogen and Nitrogen by IXS. Obvious strong features are observed on the IXS spectra of Hydrogen (Fig. 2a.) and Nitrogen (Fig. 2b). The spectra of diatomic molecules are much more complicated than the one in the monatomic molecule Helium (illustrated in Fig. 01), and more information can be obtained including different vibration modes. We are working on theoretic calculations to understand the features we observed in the experiment, and further to reveal the property of their excited states.

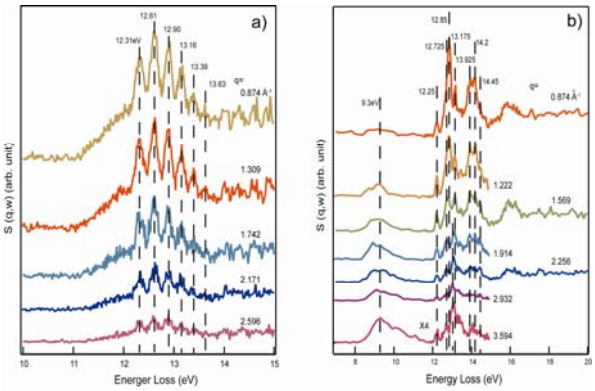

Figure 02 IXS spectra of Hydrogen (a) and Nitrogen (b).

In conclusion, we successfully applied the inelastic x-ray scattering technique to studying the electronic structure of the excited states of gas phase molecules, including monatomic molecule of Helium and diatomic molecules of Nitrogen and Hydrogen. High quality data have been obtained, and further work is on the way.

References:

[1] W. Schulke, J. Phys. Condens. Matter **13**, 7557 (2001).
[2] K. Yang *et al.*, Phys. Rev. Lett. **98**, 036404 (2007).