Study of the Li K-Edge Spectra for Various Lithium Compounds

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Abstract

The Li K-edge spectra of lithium halides, Li₂O and Li₂S have been measured and investigated by means of the molecular orbital calculation. All spectra were obtained by means of the Total Electron Yield (TEY) method, by using the ultra soft x-ray beamline 2 (BL-2) of the compact synchrotron radiation facility at Ritsumeikan University in Japan. In lithium halides, the obtained spectra are compared with the theoretical spectra calculated by the Discrete Variational (DV)- $X\alpha$ molecular orbital calculation method. The origin of the wave functions for the exciton peaks is discussed. In Li₂O and Li₂S, there are no sharp and strong peaks unlike the exciton peaks observed in the spectra for lithium halides; the shape of both the obtained spectra are very broad and similar to each other. Those spectra are also compared with the theoretical spectra and the origin of the wave function for each peak is also discussed.

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