Li K-Edge XANES Spectra of Lithium-Doped Fullerenes and Lithium Borate Glasses

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Li K-edge XANES spectra for lithium doped fullerenes, LiₓC₆₀ and LiₓC₇₀ (x = 14 ± 2), and for lithium borate glasses, xLi₂O-(100-x)B₂O₃, were measured using a beamline BL-2 of the SR Center at Ritsumeikan University [1]. All samples were powdered to collect their XANES spectra in the total electron yield mode. The vacuum level in the sample chamber was higher than 1.0 x 10⁻⁵ Pa during measurements. The lithium-doped fullerenes were synthesized at the laboratory of one of the authors (M. K.). For preparing lithium borate glasses, chemicals were melted at 1100-1200 °C and then quenched.

Figure 1 shows Li K-edge XANES spectra of LiₓC₆₀ and LiₓC₇₀ (x = 14 ± 2) and reference samples. Spectra of LiₓC₆₀ C₁ and LiₓC₆₀ C₂ show the first and second runs of the measurements of a sample LiₓC₆₀ C under Ar atmosphere, respectively. Similar measurement was done for a different sample, LiₓC₆₀ U ¹. A spectrum of LiₓC₆₀ U ² is for the sample partially exposed to the air. A spectrum of LiₓC₇₀ E ¹ is for a sample of LiₓC₇₀ measured under Ar atmosphere, and that of LiₓC₇₀ E air is for the sample exposed to the air.

Broad and somewhat split absorptions appear around 57-69 eV in the spectra of LiₓC₆₀ C ¹, LiₓC₆₀ C ², and LiₓC₆₀ U ¹, the whole features of which are similar to those of the reference samples such as Li₃N, but quite different from those of lithium halides like LiF, where the lithium atoms are in the isolated ionic states and show sharp absorption peaks due to the core exciton [2,3]. This indicates that lithium atoms in lithium-doped fullerenes do interact with C₆₀, like interacting Li and N atoms in Li₃N.

Compared to these absorptions, the corresponding broad absorption in LiₓC₇₀ E ¹ is somewhat shifted to higher energies, meaning that the Li-C₇₀ interaction is different from the Li-C₆₀ one.

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When exposed to the air, the spectral features (Li$_x$C$_{60}$ U 2 and Li$_x$C$_{70}$ E air) become similar, though the positions are a little in low energy, to those of the reference samples of Li$_2$CO$_3$ and Li$_2$O.

Figure 2 shows Li K-edge XANES spectra of lithium borate glasses xLi$_2$O-(100-x)B$_2$O$_3$ together with the reference samples. The whole spectral features of xLi$_2$O-(100-x)B$_2$O$_3$ (x = 20-45) resemble those of Li$_2$CO$_3$ and Li$_2$O. However, the spectra are rather broad with a relatively strong rising up at the low-energy side of the absorption. This may be indeed characteristic of the lithium atoms in amorphous glassy materials unlike crystalline ones.

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**References**

