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Electronic state of sulfide based solid state electrolytes applied to all solid state lithium ion secondary batteries

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All solid state batteries are expected as the next generation secondary batteries for their higher energy density, inflammable properties, and so on. In order to develop these batteries, there are several problems to improve. One of the important to improve is the ionic conductivities of the solid state electrolyte. In order to improve the ionic conductivity, electronic states of the sulfide based lithium ion conducting glasses were calculated by the DV-Xα cluster method, which is one of the first principle density functional methods. The cluster models were constructed by the coordination number reported by experimental methods and the bond length estimated from the ionic radii of each ion. The movement of the Li ion was simulated by several model clusters with different positions of the moving ion. The relationship between ionic conductivity and the differential total bond overlap population (DBOP) of the moving ion was discussed for the sulfide based glasses in the systems $Li_2S–SiS_2–Al_2S_3$ and $Li_2S–SiS_2–P2S_5$. In these glasses, the DBOP with the movement of the lithium ion had good negative correlations with the ionic conductivities and positive correlations with the activation energies obtained by the experimental measurements. In any cases, the smaller change of DBOP of the moving cations played an important role for the fast ion movement in the superionic conducting glasses. In order to search for additives with higher ionic conductivity, the composition dependence of differential total bond overlap population with addition of various fourth periodic elements to Li_2S-SiS_2 solid state electrolyte was estimated, as shown in the figure. As described above, the smaller change of the total bond overlap population with the moving Li ion makes lager ionic conductivities. The figure suggests that the addition of In, Sn and Sb to Li_2S-SiS_2 solid state electrolyte could show larger ionic conductivities. This bonding state of the moving cations is one of the characteristics of the electronic state in the sulfide based lithium ion conducting glasses.

Recent Publications

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Biography

Yoshiyuki Kowada has his expertise in structural analysis, electronic state calculation and chemical bonding analysis of amorphous materials. He applied the DV-Xα cluster method, which is one of the first principle molecular orbital calculations to the solid-state electrolytes and phosphor materials with rare earth ions. Recently, he pays attention on the study about materials to all solid state Li ion batteries for electric vehicles. He is the President of the Society for Discrete Variational Xα.

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