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Observation of π -electron in metal hexaboride through X-ray charge density

Eiji Nishibori

University of Tsukuba, Japan

Metal hexaborides MB_6 , where M is an alkaline earth or rare earth metal exhibit metallic and semiconductor properties by changing the M ion. The metal hexaborides have a B_6 octahedron in the structure. The M ion is located at the body-center surrounded by the B_6 octahedra. The B_6 octahedron has 18 valence electrons. Two electrons per B_6 octahedron are required to fulfill the bonding orbital of B_6 . Metal hexaborides with divalent metal ions are considered to be semiconductor and with the trivalent ions are metal from the consideration. Theoretical study suggests that the π -electron like an anti-bonding orbital of B_6 contributes electrical conductivity in the metallic trivalent MB_6 . We investigated the charge densities of divalent and trivalent metal hexaborides, semiconducting BaB_6 and metallic LaB_6 using the $d > 0.22$ Å ultra-high resolution synchrotron radiation X-ray diffraction data by a multipole refinement and a maximum entropy method. High resolution powder diffraction data were measured at SPring-8. The strong inter-octahedral and relatively weak intra-octahedral boron-boron bonds were observed in the charge densities. A difference of valence charge densities between LaB_6 and BaB_6 was calculated to reveal a small difference between isostructural metal and semiconductor. The weak electron lobes distributed around the inter B_6 octahedral bond were observed in the difference density. We found the electron lobes are the conductive π electrons in LaB_6 from the comparison with the theoretical charge density. We have successfully visualized very small amount of conductive π electrons from X-ray charge density. Electron density distribution is now one of the most information-rich observable owing to the great improvement of experimental situation such as synchrotron X-ray source.

Biography

Eiji Nishibori is currently a Professor of Division of Physics, Faculty of Pure and Applied Sciences, University of Tsukuba, Japan. He has received his Bachelor's and Master's degree from Nagoya University, Japan. He was appointed an Assistant and Associate Professor at Nagoya University. He was then appointed as the Director of RIGAKU-RIKEN collaboration center at SPring-8. His main research field is structural science using a synchrotron radiation X-ray including a development of experimental and analytical system. He has received several awards including Young Scientists' Prize, the Commendation for Science and Technology by the MEXT, the CrSJ Young Scientist Award and the Crystallographic Society of Japan.

nishibori.eiji.ga@u.tsukuba.ac.jp

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