Optical spectroscopy study on the electronic structure of Eu1-x Ca xB6

JUNGHO KIM, S. -J. OH, Seoul National University, YONGWOO LEE, M. G. KIM, Brookhaven National Laboratory, E. J. CHOI, University of Seoul, JONG-SOO RHYEE, B. K. CHO, Department of Materials Science and Engineering K-JIST, C. C. HOMES, Brookhaven National Laboratory — The divalent hexaboride compounds RB₆ have drawn much attention for the last decade due to their interesting electrical and magnetic properties. In EuB₆, the optical spectroscopy measurement showed an unusual shift of the plasma frequency across the ferromagnetic transition. While Ca bears no magnetic moment, CaB₆ exhibits weak ferromagnetism at high temperature. Although the band structure is a prerequisite to the understanding of these unconventional phenomena, the consensus among the theoretical and experimental works has not been reached. In this work, the optical conductivity of Eu₁₋ₓCaₓB₆ has been obtained from reflectivity and ellipsometry measurements for series of compositions, 0 < x < 1. The interband part of $\sigma_1(\omega)$ shifts continuously to higher frequency as x increases. Also the intraband spectral weight decreases rapidly and essentially vanishes for $x \geq x_c=0.35$. These results show that the valence band and the conduction band of Eu₁₋ₓCaₓB₆ move away from each other such that their band overlap decreases with increasing Ca. As a result, the electronic state evolves from the semimetallic structure of EuB₆ to the insulating CaB₆ where the two bands are separated to open a finite gap (~0.25 eV) at the X-point of the Brillouin zone.

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