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Electronic structure of $HgGa_2S_4$

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Abstract

The electronic structure and chemical bonding in HgGa2S4 crystals grown by vapor transport method are investigated with X-ray photoemission spectroscopy. The valence band of HgGa2S4 is found to be formed by splitted S 3p and Hg 6s states at binding energies BE=3–7eV and the components at BE=7–11eV generated by the hybridization of S 3s and Ga 4s states with a strong contribution from the Hg 5d states. At higher binding energies the emission lines related to the Hg 4f, Ga 3p, S 2p, S 2s, Hg 4d, Ga LMM, Ga 3p and S LMM states are analyzed in the photoemission spectrum. The measured core level binding energies are compared with those of HgS, GaS, AgGaS2 and SrGa2S4 compounds. The valence band spectrum proves to be independent on the technological conditions of crystal growth. In contrast to the valence band spectrum, the distribution of electron states in the bandgap of HgGa2S4 crystals is found to be strongly dependent upon the technological conditions of crystal growth as demonstrated by the photoluminescence analysis.