

BAND ENERGY DIAGRAM OF INDIUM BROMIDE

M.I. Kolinko, O.V. Bovgyra

Ivan Franko Lviv National University
(1, Universytetska Str., Lviv 79602, Ukraine)

S u m m a r y

Self-consistent ab initio calculations of the energy-band structure of indium bromide single crystals are performed using the norm-conserving nonlocal pseudopotential. For the first time, the energy band diagram in the \mathbf{k} -space is obtained. Optical transitions in the region of the fundamental absorption edge are identified and a good agreement with spectral measurement data is reached. The effective masses of charge carriers are calculated at some important points in the Brillouin zone. The genetic origin of certain valence bands and lower conduction bands is determined.