FIRST-PRINCIPLE CALCULATIONS OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF KCl_xBr_{1-x}, KCl_xI_{1-x} and KBr_xI_{1-x}

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ABSTRACT. Using first principles total energy calculations within the full potential linearized augmented plane wave (FP-LAPW) method, we have investigated the structural, electronic and thermodynamic properties of potassium halides (KCl_xBr_{1-x}, KCl_xI_{1-x} and KBr_xI_{1-x}), with x concentrations varying from 0% up to 100%. The effect of composition on lattice constants, bulk modulus and band gap was investigated. Deviations of the lattice constants from Vegard's law and the bulk modulus from linear concentration dependence (LCD) were observed for the three alloys. The microscopic origins of the gap bowing were explained by using the approach of Zunger and coworkers.

KEYWORDS: *FP-LAPW, potassium halides alloys, bowing gap.*