

STUDY ON THE STRUCTURAL, THERMAL AND MECHANICAL PROPERTIES OF LiCoO_2 USING FIRST PRINCIPLES METHOD

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Thin film rechargeable battery has become a research hotspot because of its small size and high energy density. Lithium cobalt oxide as a typical cathode material in classical lithium ion batteries is also widely used in thin film rechargeable batteries. In this work, structural, mechanical and thermal properties of LiCoO_2 were systematically investigated using first principles. Lattice constants, band gap and density of states were studied using Castep and VASP package, respectively. Elastic constants by applying various hydrostatic pressures between 0 to 40 GPa were computed. Specific heat and Debye temperature at low temperature were also discussed in this work. Other property including thermal conductivity was obtained using the imposed-flux method. The results show good agreement with experimental data and computational results in literature.