Ab-initio Calculations of the Phonon Density of States (DOS), Infrared (IR) and Raman Spectrum in Complex Perovskites-High Tc Superconductors

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Abstract

In present report, we have introduced a new theoretical results for LaBaCuO4, Yba2Cu4O8, Bi2Sr2CaCu2O8. By using home design programme LADY (Lattice Dynamics), we have calculated partial DOS, IR and Raman spectrums and some thermodynamics properties, like Reduced entropy and heat capacity. For example, we have observed the peaks in Raman spectrum at frequencies 3800 and 6300 cm-1 and IR active modes are condensed in frequency ranges 200-800 cm-1 in YBa2Cu4O8. The Phonon DOS are also condensed in the same frequency ranges. Also we have examined the pair distribution function, reduced entropy and reduced heat capacity for the same compounds. The isotope effect (O16 O18) in this materials is also examined and the result is presented.