

Theoretical investigation for Li_2CuSb as multifunctional materials: Electrode for high capacity rechargeable batteries and novel materials for second harmonic generation

Abstract

Based on the first-principles electronic structure calculations, we predict that Li_2CuSb should be good electrode materials for high capacity rechargeable batteries and novel materials for second harmonic generation. This prediction is based on the experimental measurements of Fransson et al. [1], and as step forward to do deep investigation on these materials we addressed ourselves for performing theoretical calculation. We found that intercalation of lithium leads to phase transitions, which agrees well with the experiment, increasing the conductivity of the material, and break the symmetry along the optical axis making the material useful for second harmonic generation (SHG) applications. We should emphasize that lithiated compound show very high second order optical susceptibility. We present the total charge densities in the (1 1 0) and (1 0 0) planes for the parent and lithiated phases and it was found that the parent compound shows a considerable anisotropy between the two planes in consistence with our calculated optical properties. We found that Li_2CuSb possesses high second harmonic generation and its second order optical susceptibility of the total absolute value at zero frequency is equal to 142 pm/V. Based on the value of the second order optical susceptibility the microscopic second order hyperpolarizability, β_{ijk} , the vector component along the dipole moment direction is about 31.01×10^{-30} esu.