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First Principles Investigation of Electronical and Lattice Dynamical Properties of High Dielectric Constant Material $Na_{1/2}Bi_{1/2}Cu_3Ti_4O_{12}$[1]

CIHAN PARLAK, RESUL ERYIGIT, Abant Izzet Baysal University, Department of Physics — We will report the results of a first principles investigation of the electronic and lattice dynamical properties of so-called giant dielectric compound $Na_{1/2}Bi_{1/2}Cu_3Ti_4O_{12}$ which was found to have a very high 'extrinsic' as well as 'intrinsic' dielectric constant. The calculations have been carried out within the local spin density functional approximation using norm-conserving pseudopotentials and a plane-wave basis. The ground state is found to be antiferromagnetic direct-band gap semiconductor. Lattice dynamical properties, such as Born effective charge tensors, dielectric permittivity tensors, and phonon frequencies at the Brillouin zone center were calculated using density functional perturbation theory and found to be similar to more studied $CaCu_3Ti_4O_{12}$ and $CdCu_3Ti_4O_{12}$ compounds. The calculated electronic ($\epsilon_\infty \approx 11.5$) and static ($\epsilon_0 \approx 150$) dielectric constants indicate that the observed high dielectric constant is extrinsic in origin. The main contribution to the static dielectric constant is found to be due to a low frequency (50 cm^{-1}) IR-active mode which has a large mode effective charge.

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