Role of the lattice dynamics in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ superconductor based on DFT method

A Tavana$^{1,2,3}$, C Ambrosch-draxl$^1$ and M Akhavan$^3$

1. Department of Atomistic Modeling and Design of Materials, University of Leoben, Leoben, Austria
2. Department of Physics, University of Mohaghegh Ardabili, Ardabil
3. Magnet Research Lab. (MRL), Department of Physics, Sharif University of Technology, Tehran
E-mail: tavana.ali@gmail.com

Abstract
Electron-phonon coupling parameters are calculated for $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ cuprate superconductor in a wide range of dopings, from undoped to overdoped compounds. In this study we aim to study the quality of such calculations based on DFT method so, the results of $\sigma$ GGA+U electronic structure calculations are also investigated. The obtained value for electron-phonon coupling is in the same order of previous calculations but, the value obtained for the Hubbard U parameter shows that, such methods are poor in the estimation of electronic correlations to decide about the role of phonons in these compounds based on their results. Moreover, existence of several structural phase transitions with temperature and doping, lead to larger error in these calculations. Based on the calculated phonon dispersions, structural phase transitions can be resulted which shows the ability of DFT in the study of structural properties and the weakness of the strongly correlations in this properties.

Keywords: cuprate superconductor, lattice structure, phase transition, electron-phonon interaction

For the full article refer to the Persian section