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Structural, electronic, linear, and nonlinear optical properties of undoped and Mo (I, II)-doped $LiNbO_3$ crystal

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Abstract. In this paper, density functional theory (DFT) calculations used to investigate the structural, electronic, linear and nonlinear optical properties of pure lithium niobate crystal ($LiNbO_3$) and doped $LiNbO_3$ by Mo (I) and Mo (I). The lattice constants were calculated by analysing the optimised unit cell, and the results were found to be in good agreement with both the experimental and theoretical values that were reported. The results indicate a clear distinction in the electronic characteristics of $LiNbO_3$ and doped $LiNbO_3$ (Mo-Nb), the band structures that have been computed indicate that the band gap of $LiNbO_3$ can be narrowed by adding Mo (I) and Mo (II) dopants to 2.068 eV and 0.476 eV, respectively. Interesting results were obtained by this doping process, as these results showed that the effect of doping led to an improvement in some optical properties, such as the absorption spectrum of the material, and also led to an increase in the effect of second harmonic generation (SHG), which is considered a basic requirement for developing optical devices in many photonic applications such as laser, electro-optic applications and optical switches.

Keyword: First Principles, Molybdenum doping, $LiNbO_3$, Electronic characteristics; Optical characteristics.

Introduction

An important family of second-order nonlinear optical materials are inorganic crystals. Additionally, it is frequently researched for a variety of photonic applications, such as resonators, filters, electro-optic, sensors, and SHG [1-3]. Due to its exceptional piezoelectric and photonic performances, the lithium-niobate (LN) is extensively utilized in commercial piezoelectric crystal materials. The LN