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The lithium doping effect for enhancing thermoelectric and optoelectronic performance of Co_2NbAl

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Cobalt-rich Heusler compounds represent a very interesting family of Heusler alloys owing to their performance in spintronics and magnetic devices [1–4]. The quaternary Heusler, created by swapping of an antiatom site with an alkali element, improves the performance of physical properties for applications [5]. In this study, the electronic structures and magnetic properties before and after substitution of Co by Li in the Co_2NbAl compound were investigated using first-principles computational calculations. At the energy plane level, the quaternary LiNbAlCo is stable and favors the cubic structure with space group of $F\bar{4}3m$ [6]. The lattice constant is in good agreement with the subsequent work [7]. Our findings revealed that substitution of Co antisites by Li destroys the half-metallic character of Co_2NbAl. Analysis of the band structures shows that the parent ternary Heusler compound is ferromagnetic half-metallic with a half-metallic ferromagnetic band gap E_{HMF} (band gap in the minority channel) and half-metallic gap G_{HM} (HM) equal to 0.22 and 0.497 eV, respectively. Our gap values are comparable to the values found by Shakeel Ahmad Sof and Dinesh C. Gupta [6]. Using the HSE06 approach substituting of Co by Li leads the material to change its behavior and becomes a semiconductor with a gap equal to 1.043 eV, this value is close to that cited in [7]. The ferromagnetic half-metallic behavior due to the $d{-}d$ exchange interaction caused by the hybridization between 3*d*-Co and 4*d*-Nb states (see the Fig. 1), where we can clearly see the contribution of the *d*-states of the transition elements Nb and Co around the fermi level. The results of optical properties such as absorption coefficient confirms that the LiNbAlCo compound has and the maximum absorption located in the middle ultraviolet (MUV 4.13–6.20 eV) region and vacuum ultraviolet (VUV 12.4–6.53 eV) region. Energy lost by an electron as it passes through the materials is given by the energy loss function $L(\omega)$ means. The largest value of $L(\omega)$ is 0.421, it is important to mention that the sharpest peaks are induced by plasmonic excitation, and the energies are considered as plasmonic energies with a value of 13.15 eV. Thermoelectric properties such as the ZT figure of merit are highly required to know the efficiency of materials that can be used in different thermal applications. The ZT for the quaternary LiNbAlCo reached 1.05 at room temperature, this value of figure of merit is very promising for the optoelectronics and encourage researchers to realize photovoltaic cells and thermoelectric generators with higher efficiency. These interesting features suggest that Co_2NbAl and LiNbAlCo Heusler compounds are good candidates for applications in spintronics and optoelectronics for commercial semiconductor industry.

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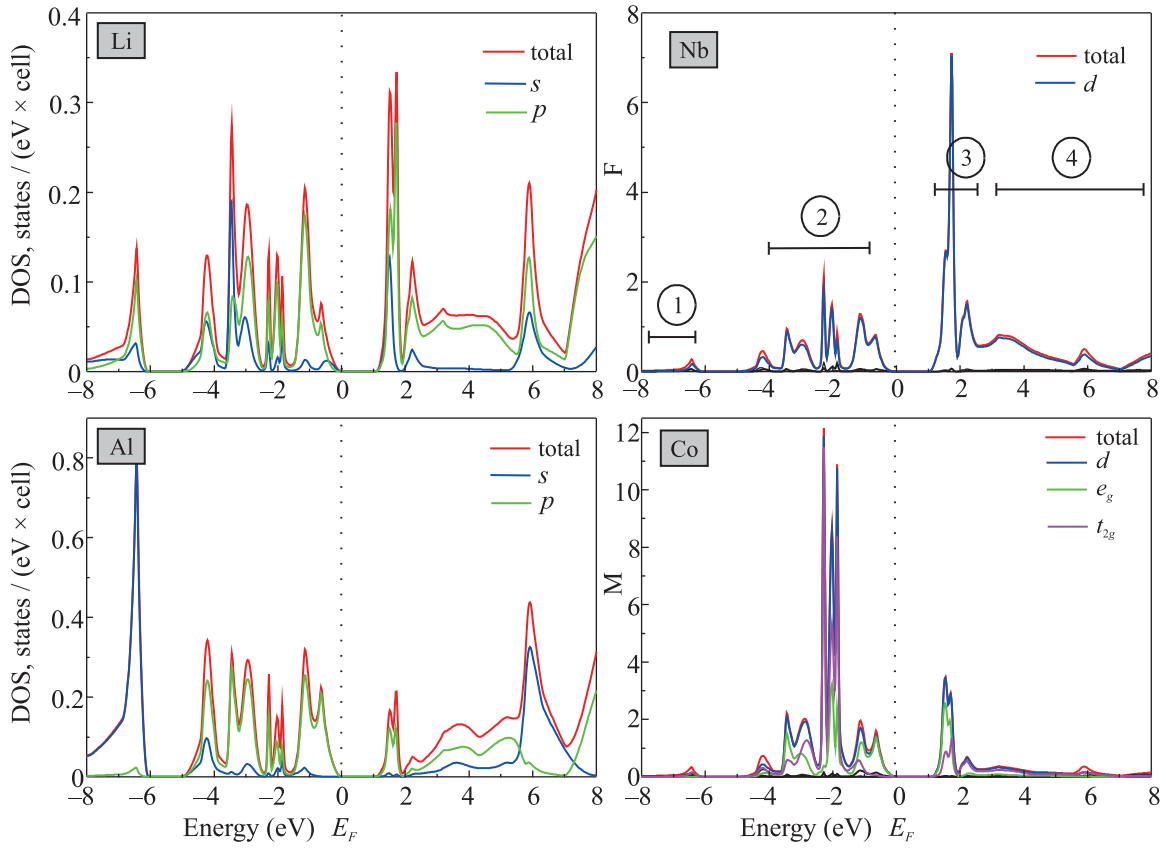

Fig. 1. (Color online) The total DOS of LiNbAlCo and the projected DOS on the states associated to Li, Nb, Al and Co

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