Study of semi metallic of LaCoO3 by density functional theory

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This thesis aims to calculate and study the electronic and optical properties of lanthanum cobaltite using the principles of the density functional theory. For this purpose, different software packages such as Wien2k and Material Studio software packages were used. In doing the calculations, the structure of the material was optimized initially and then, the electronic properties of lanthanum cobaltite were calculated through LDA and GGA approximations. The results of the approximations showed lanthanum cobaltite as a conductor with no energy gap, which is not consistent with empirical results. Then the LSDA approximation was used to examine the material. Using this approximation, the spin effect was considered in the calculations, which showed that simply considering spin effects could not predict the electronic properties of this material correctly. Namely, no energy gap was observed in the structure of LaCoO3. To solve the problem, we used the principles of strong correlation in Hubbard theory; this solution was suitable since cobalt contains d electrons and we performed electron calculations based on GGA U and LSDA U approximations. Optimizing the Hubbard correlation coefficient we managed to calculate the value of this coefficient. Using this value, 1 electron volt energy gap was obtained for lanthanum cobaltite, which corresponds precisely to the reported experimental value

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