Physical Properties Analysis of Double-Perovskite Oxide (La2CoMnO6) for Spintronics Devices: A First-Principles Density Functional Theory Study

Abu Sualmi, Rala (School: Manarat Al-Madinah National School)

La2CoMnO6 (LCMO), a transition metal double perovskite oxide, is considered a promising raw material for spintronics. Spintronics will help to develop a smaller, less energy-consuming, and higher processing capabilities device, compared to the electronic one. However, LCMO structural and physical properties that have been observed experimentally lack theoretical explanation on a quantum mechanical level, which is needed to develop a more accurate spintronic device. Therefore, this research presents a theoretical analysis of the structural and physical properties of LCMO such as magnetic and electronic properties, by using first-principles Density Functional Theory (DFT) employing Generalized-Gradient-Approximation (GGA) functional. The lattice parameter, ground-state magnetic ordering, individual atomic contribution on the magnetic moment, bandgap structure, and density of states were obtained computationally by DFT calculations on Shaheen II supercomputer. After obtaining the data from DFT, it was implemented on two quantum models: the Heisenberg model and the mean-field approximation theory to confirm the experimental and computational results. The Heisenberg model was used to obtain the coupling constants to verify the magnetic ordering, and mean-field approximation theory was used to obtain Curie temperature. The quantum models have confirmed the computational results, which match the experimental observations. It was found that LCMO has a ferromagnetic ordering with coupling constants equal to 0.014eV, 0.013eV, a half-metallic state, and 298.175 K Curie temperature. Furthermore, this study will open the door for new development in spintronics devices, leading to technological advancement in many fields, such as nanoelectronics, and quantum computing.