A DENSITY FUNCTIONAL THEORY BASED STUDY OF LANTHANUM NICKELATE

ABSTRACT

Rare-earth nickelate compounds have been a field of extensive research for many years due to some fascinating phenomena exhibited by them, such as ferroelectricity, layered structure superconductivity, and the metal to insulator transition. Lanthanum nickelate ($LaNiO_3$) is the only exception in the nickelate series which remains a paramagnetic and strongly correlated metal at all temperatures, and never undergoes a metal to insulator transition. $LaNiO_3$ finds applications in various opto-electronic, magneto-electronic, memory devices, and as catalyst in batteries and fuel cells, owing to its metallic nature. Appropriate application of $LaNiO_3$ in these various fields demands a precise control over its physical properties. Along with experimental studies, a detailed theoretical description of the physical properties of this compound and the changes they undergo in different conditions needs to be addressed thoroughly. Density functional theory (DFT) + Hubbard *U* method with suitable functional has been employed to understand how strain, oxygen vacancy and substitution of Ni by other transition metal atoms can modulate the physical properties of $LaNiO_3$. Different optical properties like dielectric function, optical conductivity, refractive and extinction coefficients, reflectance and adsorption spectra, and transport properties namely temperature variation of resistivity, Seebeck and Hall coefficients are calculated to study the changes the compound undergoes as a function of external parameters. The metallic nature of unstrained $LaNiO_3$ is evident from the density of states and band structure calculation, and also from the Drude peak in the optical conductivity spectra and the Fermi liquid behaviour of low temperature resistivity. While application of biaxial strains of different magnitudes on the system has shown an increase in the conductivity of $LaNiO_3$, a change in the oxygen content within the material triggers a metal to insulator transition. A metal to insulator transition is also seen when certain amount of Ni atoms in the compound is substituted by Fe atoms. A material exhibiting metal to insulator transition can find significant role in Mottronics, switching and memory devices. The reasons behind the increase in conductivity upon application of strain and the oxygen content dependent metal to insulator transition are explained on the basis of changes in the electronic structure of the compound within the scope of DFT. Apart from the above mentioned studies, the catalytic activity of $LaNiO_3$ is also investigated for its potential applications in fuel cells and batteries. Catalytic properties of this compound are studied by comparing the surface energies and adsorption energies for various reaction intermediates on different $LaNiO_3$ surfaces.

Key words: Density functional theory; Strain; Oxygen vacancy; Catalytic activity