Extended Abstract

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Euroscicon conference on Advanced Nanotechnology, April 18-19, 2019 Paris, France - Optoelectronic, magnetic and structural properties of double perovskite materials affecting in Nanotechnology field

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In this paper, we have investigated the structural, electronic, magnetic and optical properties of cubic double perovskite Sr2CrZrO6using the full-potential linearized augmented plane wave method (FP-LAPW), based on the density functional theory (DFT) as implemented in the WIEN2K code The term optoelectronics is a specific discipline of electronics that focuses on light-emitting or light-detecting devices. Light-emitting devices use voltage and current to produce electromagnetic radiation (i.e., light). Such light-emitting devices are commonly used for purposes of illumination or as indicator lights. In contrast, light-detecting devices, such as phototransistors, are designed to convert received electromagnetic energy into electric current or voltage. Photons are the fundamental units of electromagnetic radiation (EMR). Photons have a frequency of propagation, and we classify EMR based on this frequency-microwave EMR, infrared EMR, optical EMR, and so forth. The human eye is sensitive to optical EMR, which is further categorized into colors. Color is not an inherent property of photons; rather, photons have frequency, and human beings interpret these different frequencies as different colors Light-detecting devices can be used for light sensing and communication. Examples of these include darkness-activated switches and remote controls. In general terms, light-detecting devices work by using photons to liberate bound electrons within semiconductor materials. The exchange correlation potentials are treated by the generalized gradient approximation (GGA), GGA+U where U is on-site coulomb interaction correction as well as modified Becke-Johnson (mBJ) which have been used to correct the potential. Calculations were performed with the Birch-Murnaghan approach to determine the equilibrium phase, lattice, bulk modulus and its pressure derivative. The results display a half-metallic ferromagnetic ground state for the cubic double perovskite Sr2CrZrO6 compound due to the strong correlation effect of transition metal Cr(3d-t2g) states with the integer value of the total magnetic moment. Furthermore, we found a direct gap (Γ-Γ) around the Fermi level, making this material. A large number of optoelectronic devices consist of a p-type and n-type region, just like a regular p-n diode. The key difference is that there is an additional interaction between the electrons and holes in the semiconductor and light. This interaction is not restricted to optoelectronic devices. Regular diodes are also known to be light sensitive and, in some cases, also emit light. The key difference is that optoelectronic devices such as photodiodes, solar cells, LEDs and laser diodes are specifically designed to optimize the light absorption and emission, resulting in a high conversion efficiency. In multiferroic materials, a stable electric polarization can be controlled by applying an external magnetic field and vice versa, as mediated by the magnetoelectric (ME) coupling. Such a unique property makes these systems extremely useful for many technological applications ranging from tunable multifunctional spintronics to magnetoelectric random access memory devices and many kinds of optoelectronic devices. Physically, as pointed out by Aizu and later on by other authors, the ME coupling between magnetism and ferroelectricity is governed by a simultaneous breaking of inversion and time-reversal symmetries. Since its first prediction, the search for multiferroic materials, has become one of the most active research areas in condensed matter and material physics.

Note: This work is partly presented at Euroscicon conference on Advanced Nanotechnology, April on 18-19, 2019 held at Paris, France

Furthermore, most ferromagnets are metallic with half-filled d-bands, while ferroelectrics are insulating with fully filled d-bands, which makes it more difficult to find a suitable multiferroic. So far, the transition-metal oxides BiFeO310–13 and RMnO3 (where R for rare-earth elements) are candidates for multiferroics. Unfortunately, none of these single-phase perovskite materials demonstrate significant and robust electric and magnetic polarizations at room temperature. Currently, there is a lot of experimental and theoretical interest in the possibility of tuning the magnetism of these multiferroic materials by placing them in contact with other transition-metal oxides (TMOs). There are two lines of effort toward this goal: One way is to form an interface between one of these multiferroic materials and another type of TMOs. The interface platform has proved to be successful in generating novel emergent states that are nonexistent in its constituent TMO bulk. Another way is to form a three-dimensional mesoscale structure, in which one constituent TMO plays the role of a matrix and the other serves as a pillar. Toward the understanding of the coupling mechanism in these heterostructure materials, the ordered double perovskite Bi2FeMnO6 (BFMO), which can be regarded as an extreme case of particular-matrix heterostructure, is particularly interesting, with the potential of improved electric and magnetic properties. Experimentally, the BFMO can be synthesized (see experimental method) through the dilution of the Fe-sublattice by Mn in BiFeO3 while the end member BiMnO3, isostructural to BFeO3, is ferromagnetic below ?105 K.8,23 Earlier studies of BFMO thin films reported a weak enhancement of moment of a magnet up to ?0.18 μB/f.u. at 10 K for thickness 65–85 nm;24 while only a tiny magnetic moment less than 0.01 μB/f.u. was observed at 5 K for thickness ?220 nm.25 More recently, the measurements on strained thin films (thickness ?30 nm) by Choi et al.6 have shown a large magnetic moment of ?1.16 μB/f.u. at room temperature. The significant difference of the magnetic moment on much thinner and thick films originates from the fact that the much thinner thin films are highly strained and tetragonal.

Light absorption and emission in a semiconductor is known to be heavily dependent on the detailed band structure of the semiconductor. Direct bandgap semiconductors, i.e semiconductors for which the minimum of the conduction band occurs at the same wavevector, k, as the maximum of the valence band, have a stronger absorption of light as characterized by a larger absorption coefficient. They are also the favored semiconductors when fabricating light emitting devices. Indirect bandgap semiconductors, i.e. semiconductors for which the minimum of the conduction band does not occur at the same wavevector as the maximum of the valence band, are known to have a smaller absorption coefficient and are rarely used in light emitting devices.

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