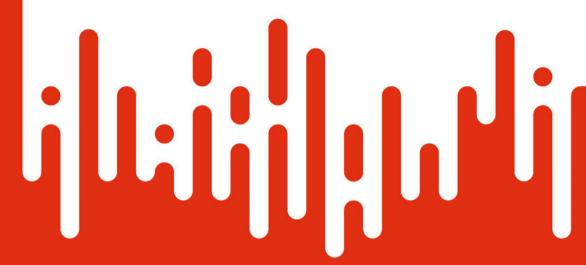
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Rachid Masrour



Magnetoelectronic,
Optical, and
Thermoelectric
Properties of Perovskite
Materials



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Rachid Masrour

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General Introduction

The perovskite oxide is a versatile class of compounds with A-site being 12 coordinated and occupied by rare earth or alkaline earth ions with large ionic radii. The B-site being octahedrally coordinated and generally occupied by a transition metal ion or rare earth ion with smaller ionic radii. It contains corner sharing BO₆ octahedra and the voids are filled by the larger radius A cations. Perovskite solar cells have attracted extensive attention due to their excellent optoelectronic properties, low cost, and easy fabrication, among other qualities [1–3]. Because of lead's high toxicity for the environment and humans, the industrial application of lead-based perovskites has been greatly limited [4, 5]. Currently, perovskite solar cells hold a record efficiency of 25.6% in a laboratory scale [6]. For organic-inorganic hybrid perovskites, secondary growth is usually achieved by a post-synthetic treatment induced in-situ transformation to perovskites with reduced dimension and higher stability, especially along the defect-rich grain boundaries [7]. Inorganic perovskites, exemplified by CsPbI₃, are characterized by superior chemical stability compared to their organic A-site cation counterparts. However, they do exhibit a higher density of defects. Nevertheless, achieving an organized secondary arrangement or reconstruction in these inorganic perovskites with reduced defects presents a significant challenge due to their distinctive chemical properties [8]. The performance of perovskite photodetectors has made a breakthrough in a short time. At present, the perovskite photodetectors with external quantum efficiency over 90% have been realized [8], and the external quantum efficiency (EQE) can be further enhanced by introducing photomultiplication (PM) effect. Moreover, some special properties, such as oxygen vacancies and the change in the B-site ion valence state, will significantly influence the catalytic activity of these perovskite materials [9]. Additionally, perovskite oxides can be made into different types of sensors, e.g., current and capacitance sensors, which are based on their various electrochemical properties such as good conductivity and dielectric properties [10, 11]. The research in the area of A-site ordering of this family of double perovskites is less compared to the B-site ordering. The result of these rare studies of A-site ordering is particularly due to the fact that most of the materials with these sorts of ordering needs high pressure synthesis and exist over a very narrow range of temperature [12–14]. Previous studies have shown that vi General Introduction

La₂NiTiO₆ and La₂MnTiO₆ exhibit long-range paramagnetism at room temperature, which can explain laterally that Ti does not exhibit antiferromagnetism macroscopically in the double perovskite system, eliminating the risk of introducing additional antiferromagnetic particles [15, 16]. Previous researchers have found many interesting properties in halide perovskites [17–19], due to their complicated structure and noncentral symmetry, especially when transition metal (TM) ions are incorporated or used [20–22]. Recently, chalcogenide perovskites have received increased attention as an emerging ionic semiconductor family with fascinating optoelectronic properties [23–28]. The electronic, magnetic and magnetocaloric properties of $T_{1-x}Sr_xMnO_3$ with (T=La, Pr) and (x = 0.35 and 0.25) were studied by using the density functional theory and Monte Carlo study with the generalized gradient GGA, GGA+U (Hubbard parameter) and the Modified Becke-Johnson approximation. The Monte Carlo simulations were used to calculate some magnetic parameters such as the exchange coupling constants and magnetic moments. The electronic, optical, thermoelectric, magnetic, and magnetic properties of the GdCrO₃ system by using the DFT and Monte Carlo simulation. We have studied the magnetic properties and magnetocaloric effect in Sr₂FeMoO₆, La₂SrMn₂O₇ bilayer manganite, the surface effects on the magnetocaloric properties of perovskites ferromagnetic thin films, $SmFe_{1-x}Mn_xO_3$ perovskite.

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