The modeling of optical and magneto-optical properties of $La_{1-x}Sr_xMnO_3$ from first principles

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The $La_{1-x}Sr_xMnO_3$ with composition about x=0.3 is presently considered as prototype and reference material (LSMO) for hole doped manganite perovskites in the studies of different mechanisms underlying unusual properties of these compounds and the potential technological usefulness of their colossal magnetoresistance. The magneto-optical properties of LSMO yield information about the spin-dependent electronic structure of the material [1, 2]. In the present work, the optical and magneto-optical properties of LSMO have been studied from *ab-initio* spin-polarized linear muffin-tin orbital relativistic band structure calculations by the local spin-density approximation (LSDA)+*U* method [3]. As the influence of different factors on the electronic properties of the manganite perovskites is still the subject of discussion, we have modeled these properties by studying the role of i) the Jahn-Teller distortion of MnO_4 octahedra, ii) the substrate induced tensile and compressive strains in thin films and iii) the electronic correlations described by the Coulomb *U* on-site repulsion and exchange *J* parameters in the LSDA+*U* approach. The calculations have been performed for $La_{0.75}Sr_{0.25}MnO_3$ structure with *R*$\underline{3}$*c* symmetry and rhombohedral lattice distortion. The modeling allows establish relative importance of these effects and mechanisms, and the results of the calculations have been successfully compared with the experimental data. The effect of the lattice distortion plays a key role, but the correlation effects described by *U*=1.3 eV and *J*=0.9 eV on Mn sites are of lesser significance. The results show that the LSDA+*U* approach correctly describes the excited-state properties of manganite perovskites materials.

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