Title: First-principles assessment of multifunctional ferromagnetic A_2TiCrO_6 (A = Mg, Ca, Sr, Ba, Ra) double perovskites: Physical and magnetic properties for opto-spintronic applications

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Abstract: This study investigates the physical properties of the double perovskite oxide series A_2TiCrO_6 (A = Mg, Ca, Sr, Ba, Ra) using different exchange-correlation functionals based on density functional theory (DFT). Structural stability of the A_2TiCrO_6 compounds at the equilibrium lattice constant ensures the cubic $Fm\bar{3}m$ symmetry through analyses of tolerance factors, while the Birch-Murnaghan equation reveals that the ferromagnetic (FM) phase is energetically preferred over the non-magnetic (NM) configuration. The spin-polarized electronic band structure and density of states (DOS) demonstrated that all compounds under investigation are half-metallic with nearly integral magnetic moments of 2 μ_B. The PDOS analysis indicates that the valence band is dominated by O-2p orbitals, while Ti-d states prevail in the conduction band near the Fermi level. All the compounds satisfy Born stability criteria and the ductile nature of the materials was demonstrated through Poisson's, Pugh's ratios, and Cauchy's pressure. The dynamical stability of these compounds is demonstrated through phonon dispersion curves. In thermodynamic properties, the high melting temperature and specific heat capacities demonstrate that the investigated compounds are thermally suitable for high-temperature device applications. Optical analyses show that the static refractive index exceeds unity and aligns well with predictions from the Penn model. Furthermore, the absorption, refractive index, extinction coefficient, and optical conductivity spectra suggest that these compounds are suitable for UV-based optoelectronic applications. The electronic, optical, mechanical, and magnetic properties suggest that these materials are promising candidates for spintronic applications. Moreover, the coexistence of high spin polarization, a tunable dielectric response, and strong UV optical activity establishes the A2TiCrO6 compounds as multifunctional materials suitable for spintronic and optoelectronic applications.

Keywords: Spin-polarizationOptoelectronicsPhotocatalyticHalf-metallicitySpintronicsDFT

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