INTERNATIONAL JOURNAL OF
ENERGY RESEARCH

RESEARCH ARTICLE

Structural, electronic, elastic, and magnetic properties of $NaQF_3$ (Q = ag, Pb, Rh, and Ru) flouroperovskites: A first-principle outcomes

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First published: 26 September 2021 | https://doi.org/10.1002/er.7319

Summary

This study presents some physical properties of fluoroperovskite NaQF3 (Q = Ag, Pb, Rh, and Ru) compounds computed with the help of the first-principle study. Fundamental structural features, ie, basic structural parameters, are investigated and reported, including the lattice constant, bulk modulus, and its pressure derivative. The compounds of interest are founded to be structurally stable. The Goldschmidt's tolerance factor (τ) is an indicator for the stability and distortion of perovskites crystal structures; it is found that τ is 0.951 for $NaAgF_3$, 0.954 for $NaPbF_3$, 0.934 for $NaRhF_3$, and 0.971 for $NaRuF_3$; therefore, NaQF3 (Q = Ag, Pb, Rh, and Ru) are stable fluoroperovskites. Elastic properties are computed, and it is examined that all the compounds are elastically stable, anisotropic, and ductile. For all these materials, the electronic band structure and density of states in both spin-up and spin-down schemes are simulated and presented. In the spin-up scheme of NaAgF3 material, an indirect bandgap of 2.54 (eV) exists from M -Γ, while in the spin-down scheme, NaAgF3 has no bandgap. Bandgap of 1.44 (eV) for NaRhF3 exist in spin-down configuration and an overlapping pattern in spin-up case, which confirms the spin-polarized behavior at the Fermi level. The electronic band's scheme for NaPbF3 and NaRuF3 shows that there is a bandgap in NaRuF3 of 2.37 (eV), which is indirect from M -Γ in both (spin-up and spin-down) cases, thus depicting a semiconducting nature. In NaPbF3, the spin-up and -down scheme manifests a metallic behavior. In summarizing the electronic band structures, it is noted that NaAgF3 and NaRuF3 show a 100% spin-polarized nature at the Fermi level, and are half-metallic. NaPbF3 represents metallic and $NaRuF_3$ represents a semiconducting behavior. Selected studied compounds are found and classified as ferromagnetic because of the total integer value of the magnetic moments. WIEN2k code is employed for these computations, in which the full-potential linearized augmented plane wave (FP-LAPW) approach is used within density functional theory (DFT). To treat and perform the total energies calculations, the exchange-correlation potential of generalized gradient approximation with the additional Hubbard-U term for indulging on-site Coulomb interaction (GGA + U) is considered. Based on a precise and good outcome for the reported compounds, beneficial applications in electronic and magnetic technology can be predicted from the electronic and magnetic properties.