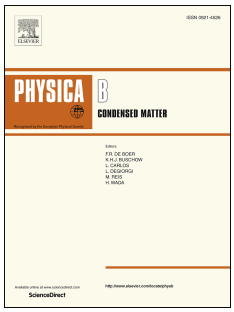
Accepted Manuscript



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PII: S0921-4526(18)30159-5

DOI: 10.1016/j.physb.2018.02.039

Reference: PHYSB 310756

To appear in: *Physica B: Physics of Condensed Matter*

Received Date: 13 December 2017

Revised Date: 23 February 2018

Accepted Date: 24 February 2018

Please cite this article as: S. Ali, M. Rashid, M. Hassan, N.A. Noor, Q. Mahmood, A. Laref, B.U. Haq, Ab-initio study of electronic, magnetic and thermoelectric behaviors of LiV_2O_4 and $LiCr_2O_4$ using modified Becke-Johson (mBJ) potential, *Physica B: Physics of Condensed Matter* (2018), doi: 10.1016/j.physb.2018.02.039.

Ab-initio study of electronic, magnetic and thermoelectric behaviors of LiV_2O_4 and $LiCr_2O_4$ using modified Becke-Johson (mBJ) potential

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Abstract

Owing to the large energy storage capacity and higher working voltage, the spinel oxides LiV_2O_4 and $LiCr_2O_4$, have remained under intense research attention for utilization as electrode materials in lithium-ion batteries. In this study, we explore the half-metallic nature and thermoelectric response in both LiV_2O_4 and $LiCr_2O_4$ spinel oxides using *ab-initio* density functional theory (DFT) based computations. The ground-state energies of these compounds have been studied at the optimized structural parameters in the ferromagnetic phase. In order to obtain a correct picture of the electronic structure and magnetic properties, the modified Becke-Johnson (mBJ) potential is applied to compute the electronic structures. The half-metallic behavior is confirmed by the spin-polarized electronic band structures and density of state plots. The magnetic nature is elucidated by computing the John-Teller energy, direct and indirect exchange and crystal field splitting energies. Our computations indicate strong hybridization decreasing the V/Cr site magnetic moments and increasing magnetic momenta at the nonmagnetic atomic sites. We also present the computed parameters significant for expressing the thermoelectric response, which are electrical conductivity, thermal conductivity, See-beck coefficient and power factor. The computed properties are of immense interest owing to the potential spintronics and Li-ion battery applications of the studied spinel materials.

Keywords:

Ab-initio calculations, half-metallic spinel oxides, magnetic properties, thermoelectric properties