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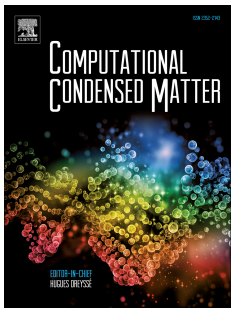

Ab-initio prediction of half-metallicity in Lithium chalcogenides compounds LiX (X=S, Se and Te) in zinc-blende and wurtzite structures

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Ab-initio prediction of half-metallicity in Lithium chalcogenides compounds LiX (X=S, Se and Te) in zinc-blende and wurtzite structures

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Abstract:

The first-principles full-potential linearized augmented plane-wave method (FPLAPW) based on density functional theory (DFT) is used to investigate electronic, structural and magnetic properties of LiX (X=S, Se and Te) binary compounds in assumed five types of crystalline structures (rocksalt (B1), CsCl (B2), ZB (B3), WZ (B4) and NiAs ($B8_1$)). Using the generalized gradient approximation of Perdew, Burke, and Ernzerhof (GGA-PBE), we find that, due to the spin polarized *p* orbitals of group VI elements, ZB and WZ LiS and ZB LiSe are half-metallic ferromagnets with an integer magnetic moment of 1 μ_B per formula unit. However, by using mBJ-GGA-PBE the three compounds LiS, LiSe, and LiTe in the ZB and WZ structures are half-metallic ferromagnets with an integer magnetic moment of 1 μ_B per formula unit. In all the cases and for the three Li based compounds, the ferromagnetic phase is energetically favored with respect to the paramagnetic one, expect for LiS compound in NiAs structure, its paramagnetic phase is energetically favored with respect to the ferromagnetic.

Keywords: DFT, Half-metals, Ferromagnetism, Alkali metals, Chalcogenides.

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