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Investigation insights into electronic structures, exchange splittings, induced ferromagnetism and half-metallic feature in new Ti-doped BaS

B. Doumi[+*1)], *A. Mokaddem*[*×1)], *A. Tadjer*[°]

[+]*Faculty of Sciences, Department of Physics, Dr. Tahar Moulay University of Saida, 20000 Saida, Algeria*

[*]*Instrumentation and Advanced Materials Laboratory, University Center of Nour Bachir El-Bayadh, 32000 El-Bayadh, Algeria*

[×]*University Center of Nour Bachir El-Bayadh, 32000 El-Bayadh, Algeria*

[°]*Modelling and Simulation in Materials Science Laboratory, Physics Department, Djillali Liabes University of Sidi Bel-Abbes, 22000 Sidi Bel-Abbes, Algeria*

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The new $Ba_{1-x}Ti_xS$ compounds based on the titanium (Ti)-doped BaS at various concentrations $x = 0.25$, 0.5 and 0.75 were characterized using the first-principle concepts of density functional theory. We investigated the doping effect of titanium on the structural and electronic properties, induced ferromagnetism, half-metallicity and exchange splittings in $Ba_{1-x}Ti_xS$ materials. The generalized gradient approximation of Wu and Cohen is employed to compute structural properties, while the Tran–Blaha modified Becke–Johnson potential is used to determine magnetic properties and electronic structures with perfect gaps.

The origin of ferromagnetism in the $Ba_{1-x}Ti_xS$ compounds is due to the localized partially occupied 3d (Ti) states related to the double exchange mechanism. The electronic structures of $Ba_{1-x}Ti_xS$ at concentrations $x = 0.25$ and 0.5 show half-metallic ferromagnetic character with spin polarization of 100 %. For concentration $x = 0.75$ the $Ba_{0.25}Ti_{0.75}S$ exhibits a metallic nature for two spins channels due to widening 3d (Ti) states in the gap. Therefore, $Ba_{1-x}Ti_xS$ at concentrations $x = 0.25$ and 0.5 seems to be potential candidates for spintronics.

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[1)]e-mail: bdoummi@yahoo.fr, mokaddem.allel@gmail.com; author's ORCID ID: http://orcid.org/0000-0003-1563-8587