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Variety of spin-polarization in the Gd-Sb compounds

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Speaker: Baidak Semyon Timofeevich

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Crystal structure

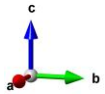

Gd

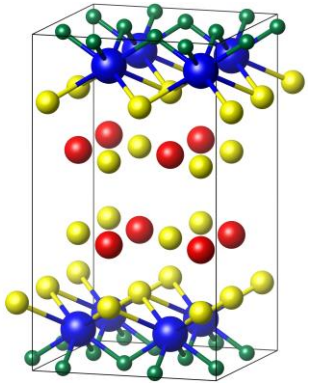

Sb


S


O

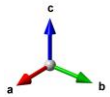
(a)

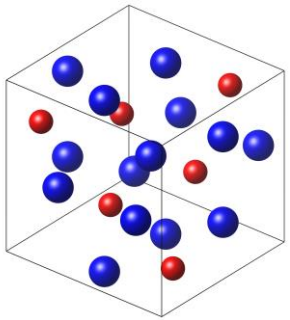




$GdSbS_2O$

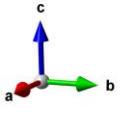
(b)

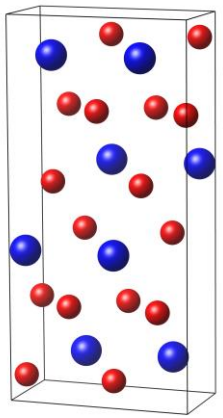




Gd_4Sb_3

(c)





$GdSb_2$

Lattice parameters

Compound	Space Group (No.)	Lattice Parameters (Å)		
		a	b	c
$GdSbS_2O$	129	3.900	3.900	13.700
Gd_4Sb_3	220	9.220	9.220	9.220
$GdSb_2$	64	6.157	5.986	17.830

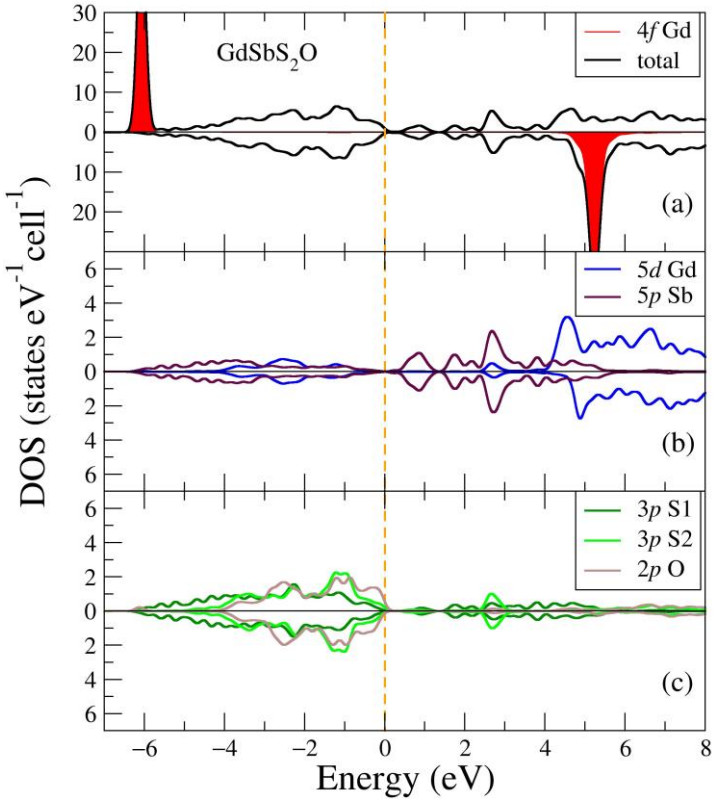
Computational method

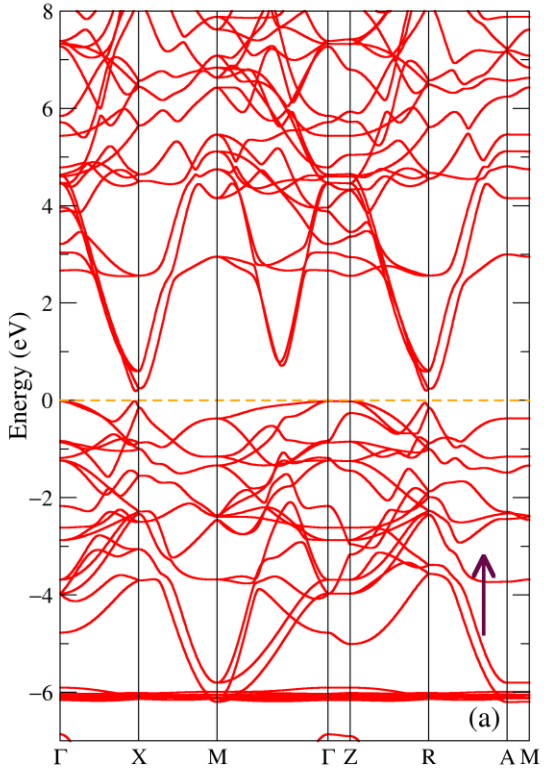
Electronic structure calculations were conducted in Quantum Espresso package [1] using GGA+U version of LSDA+U method [2]. The exchange correlation potential was employed in generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) [3].

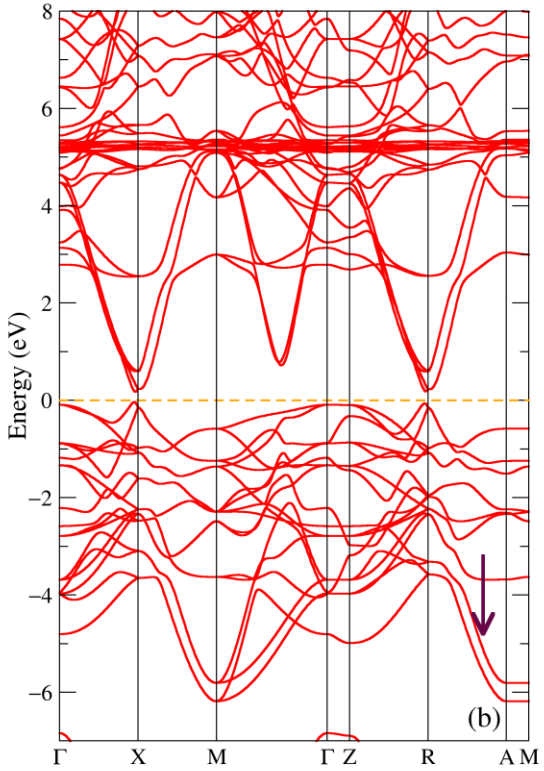
Hund's exchange parameter for Gd: **J = 0.7 eV**.
Direct Coulomb interaction for Gd: **U=6.7 eV** [4].

[1] J. Phys.: Condens. Matter. 21, 395502 (2009).
[2] Phys. Rev. B 44, 943 (1991).
[3] Phys. Rev. Lett. 77, 3865 (1996).
[4] J. Phys. Condens. Matter, 9, 767–808 (1997).

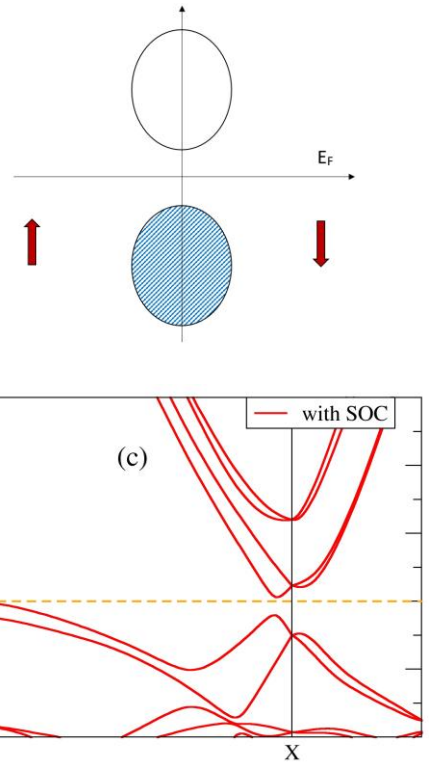
Electronic structure of $GdSbS_2O$







semiconductor

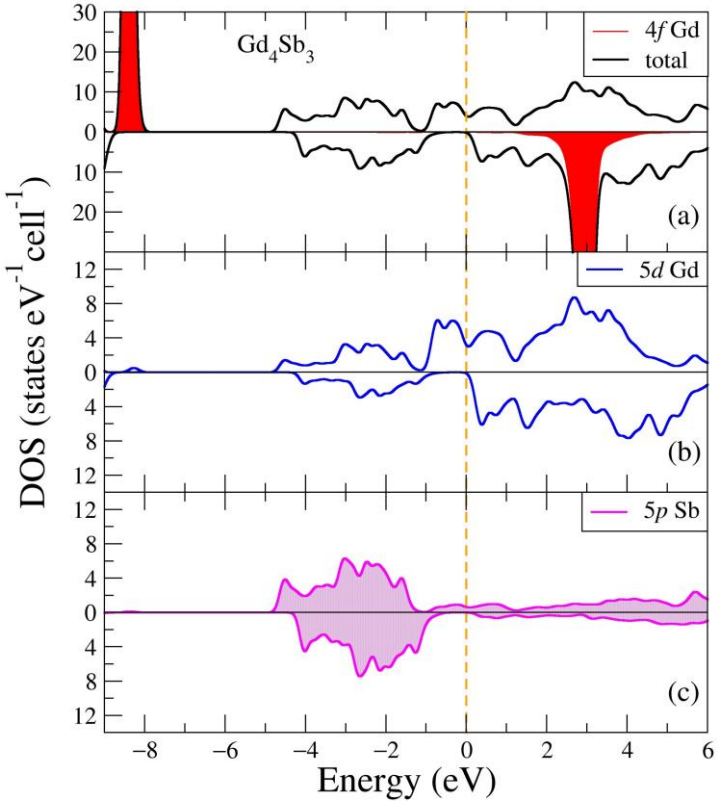


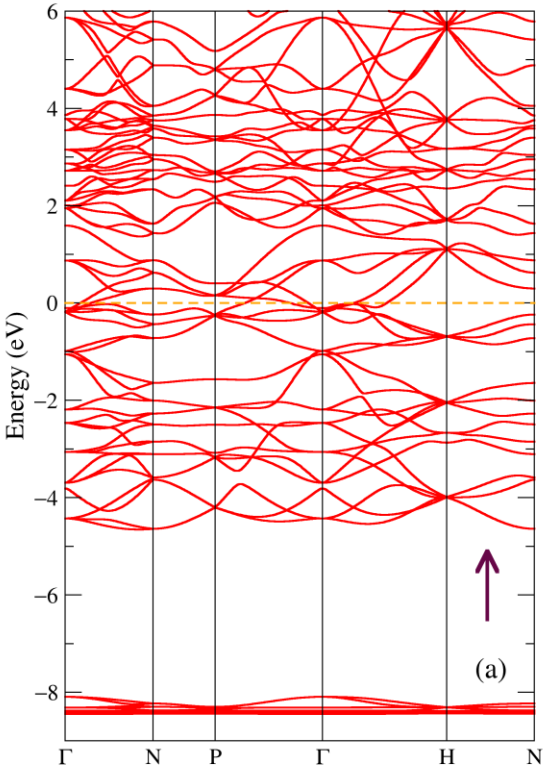
$E_{g\uparrow} = E_{g\downarrow} = 0.2\ eV$ $E_{g(SOC)} = 0.03\ eV$

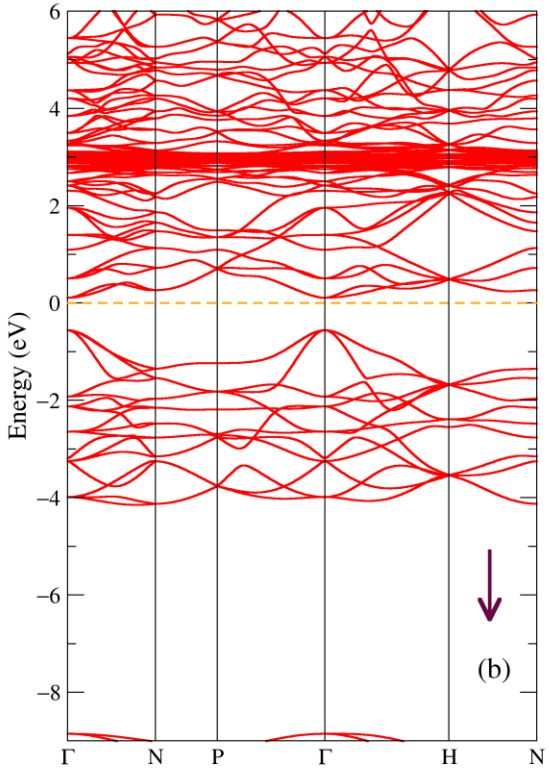
It turns out that $GdSbS_2O$ is a semiconductor with a narrow indirect gap between points Γ and X.

Spin-polarization value equals to 0%.

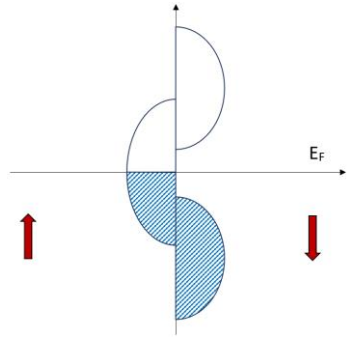
Electronic structure of Gd_4Sb_3



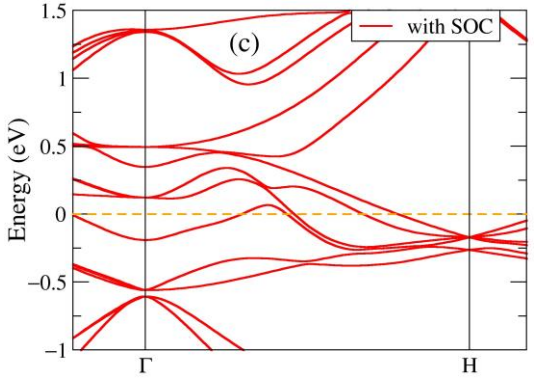




half-metal

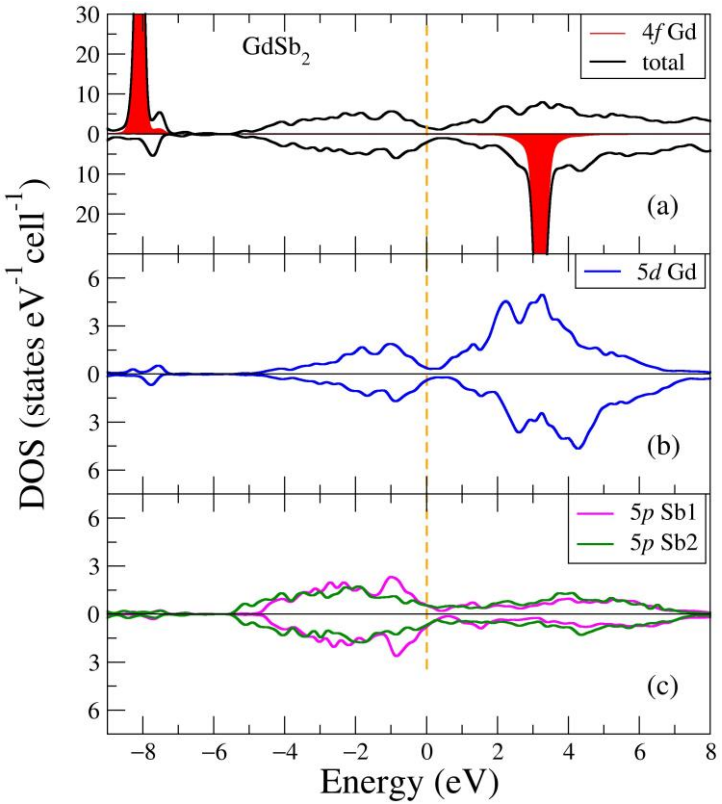


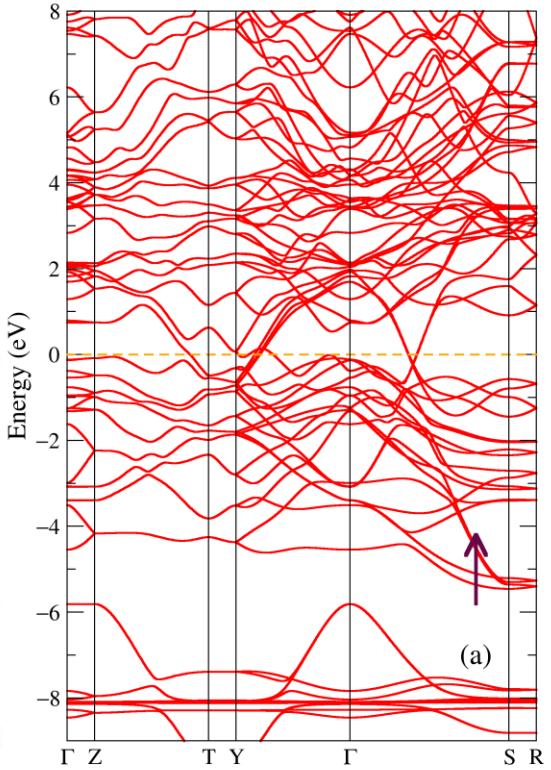
$E_{g\downarrow} = 0.67\ eV$

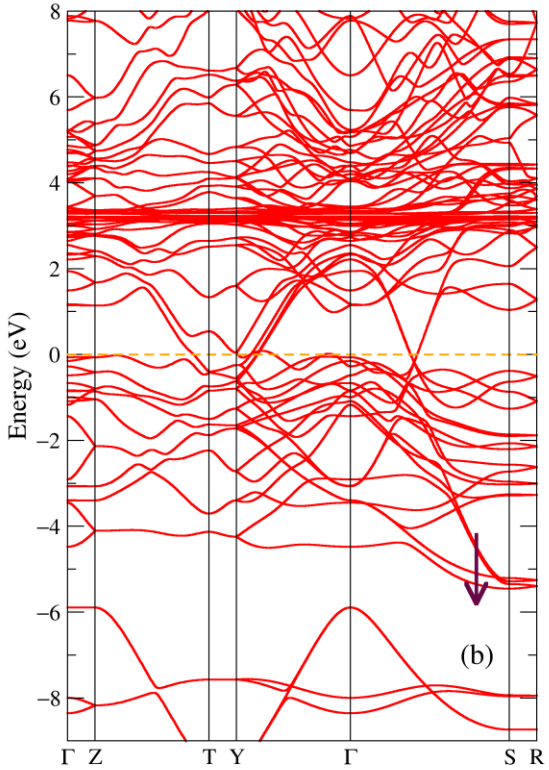


The energy gap is present only for the minority spin projection, the other spin projection shows metallic nature and thus Gd_4Sb_3 is a half-metal. Spin-polarization value is 100%.

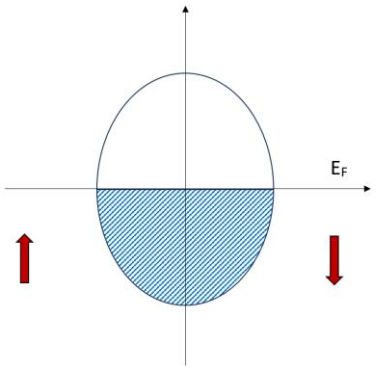
Electronic structure of $GdSb_2$

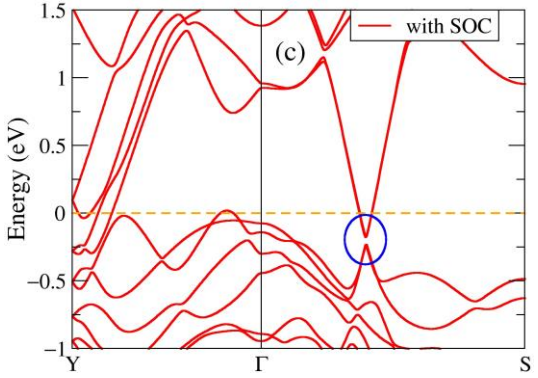






metal





Valence and conduction bands overlap which is typical for metals. Spin-polarization value is 11.3%.

Conclusions

Electronic structure of the compounds has been studied
$GdSbS_2O$ is a narrow gap semiconductor with the gap value of 0.03 eV
We conclude that Gd_4Sb_3 is a half-metal
$GdSb_2$ exhibit metallic properties
The results are published in S.T. Baidak, A.V. Lukoyanov, Semimetallic, Half-Metallic, Semiconducting, and Metallic States in Gd-Sb Compounds, Int. J. Mol. Sci., 24, 8778 (2023)

Compound	Spin-polarization value
$GdSbS_2O$	0%
Gd_4Sb_3	100%
$GdSb_2$	11.3%

RSF Russian Science Foundation

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Thank you for your attention