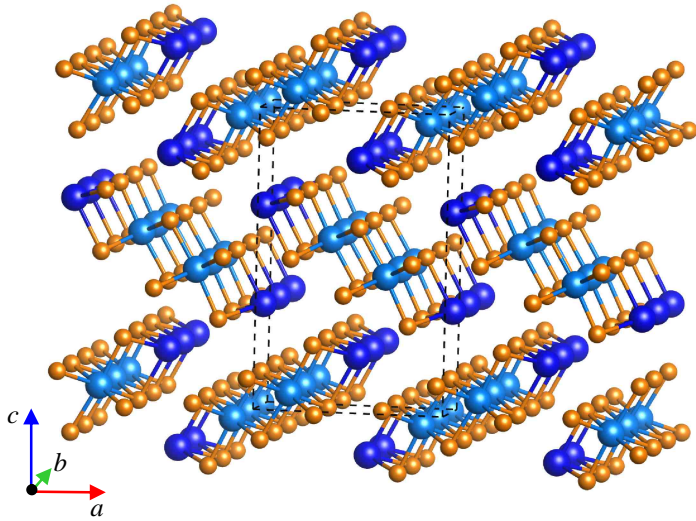


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... , ... , 88000, ... , 54  
 e-mail: crystal\_lab457@yahoo.com

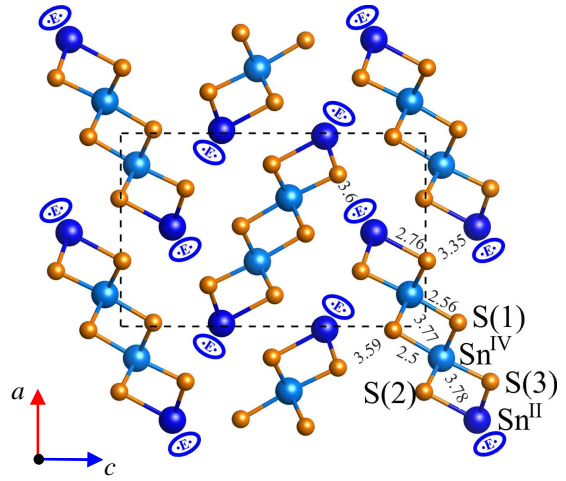
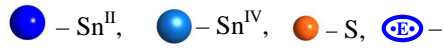
### Sn<sub>2</sub>S<sub>3</sub>

Sn<sub>2</sub>S<sub>3</sub>; ...  
 Sn<sub>2</sub>S<sub>3</sub> ...  
 $E_{gi} = 0.53$  ...  
 S3p- ...  
 S-Sn ...  
 Sn<sub>2</sub>S<sub>3</sub> ...  
 Sn-S ...  
 SnS, SnS<sub>2</sub>, ...  
**1.** ...  
 Sn<sub>2</sub>S<sub>3</sub> ...  
 β-, γ- δ- ...  
 [2]. ...  
 (Sn<sub>2</sub>S<sub>3</sub>) ...  
 [3], ...  
 [4, 5], ...  
 [6], ...  
 Sn<sub>2</sub>S<sub>3</sub> [7]. ...  
 Sn<sub>2</sub>S<sub>3</sub> ...  
 [8], ...  
 $E(\mathbf{k})$  ...  
 Sn<sup>II</sup>, ... Sn<sup>IV</sup> ... S ( ... 2).  
 Sn<sup>II</sup> ... Sn<sup>II</sup> Sn<sup>IV</sup> ...  
 Sn<sup>IV</sup> ...  
 S(1), S(2) S(3) ...  
 4 ...  
 m ( ... 1, ...).  
*ab initio* ...  
*Pnma*



. 1.

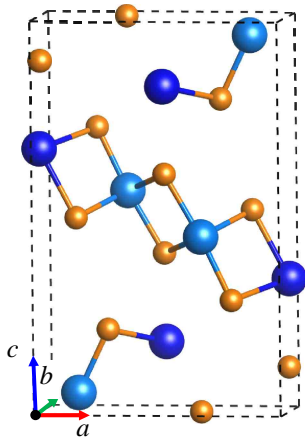
( )



XZ ( )

Sn<sub>2</sub>S<sub>3</sub>

2.



. 2.

Sn<sub>2</sub>S<sub>3</sub>.

Sn<sup>II</sup> 5p-

5s-

(ABINIT),

(SIESTA),

[12–15],

[16, 17].

[18]

Sn – [Kr] 5s<sup>2</sup>5p<sup>2</sup>,  
[Ne] 3s<sup>2</sup>3p<sup>4</sup>.

:

S –

, [Kr], [Ne] –

[19].

3.

3.1.

ψ- [SnS<sub>3</sub>•E•], •E• –

Sn<sub>2</sub>S<sub>3</sub>  
[Sn<sup>IV</sup>S<sub>6</sub>],

b.

ψ- [SnS<sub>3</sub>•E•].

( . 3).  
Sn<sub>2</sub>S<sub>3</sub>

. 4,

E(k)

52

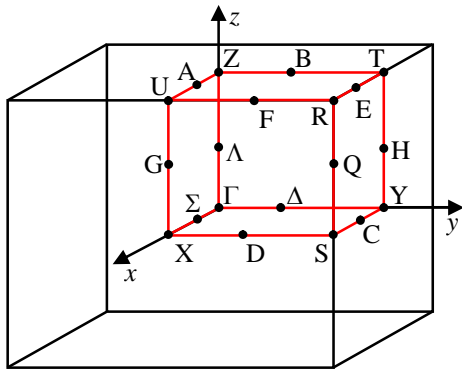


Fig. 3. Crystal lattice of  $\text{Sn}_2\text{S}_3$ .

5s-, 5p-  
 U.  
 $E_{gi} = 0.53$  ( $\rightarrow$ U).

Z ( $E_{gd} = 0.54$ ).

**3.2.**

(.5) s-, d-  
 d- s-

$\text{Sn}_2\text{S}_3$  (.5).  $\text{Sn}_2\text{S}_3$   $S3s$ -

Sn S (.5) s-, p-, d-  
 s- p-

5s- 5-  
 3 -

-14.58 -12.07 ,  
 3s- Sn 5p- 5d-

(-8.43 ÷ -5.24 ) 3s-  
 3.64 3 -  
 5s-

( -5.87 ) 5s- 3p-  
 3 - 5p-

$\text{Sn}_2\text{S}_3$ , [7],

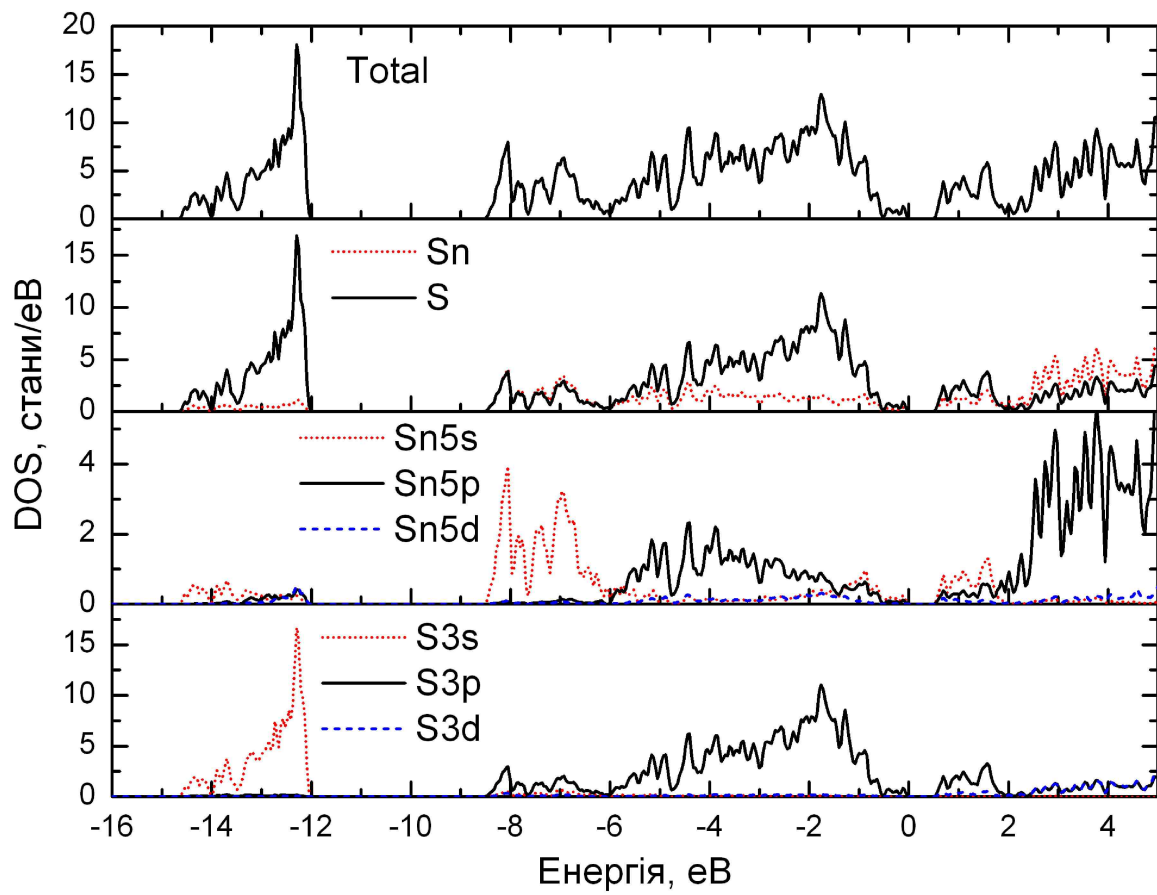
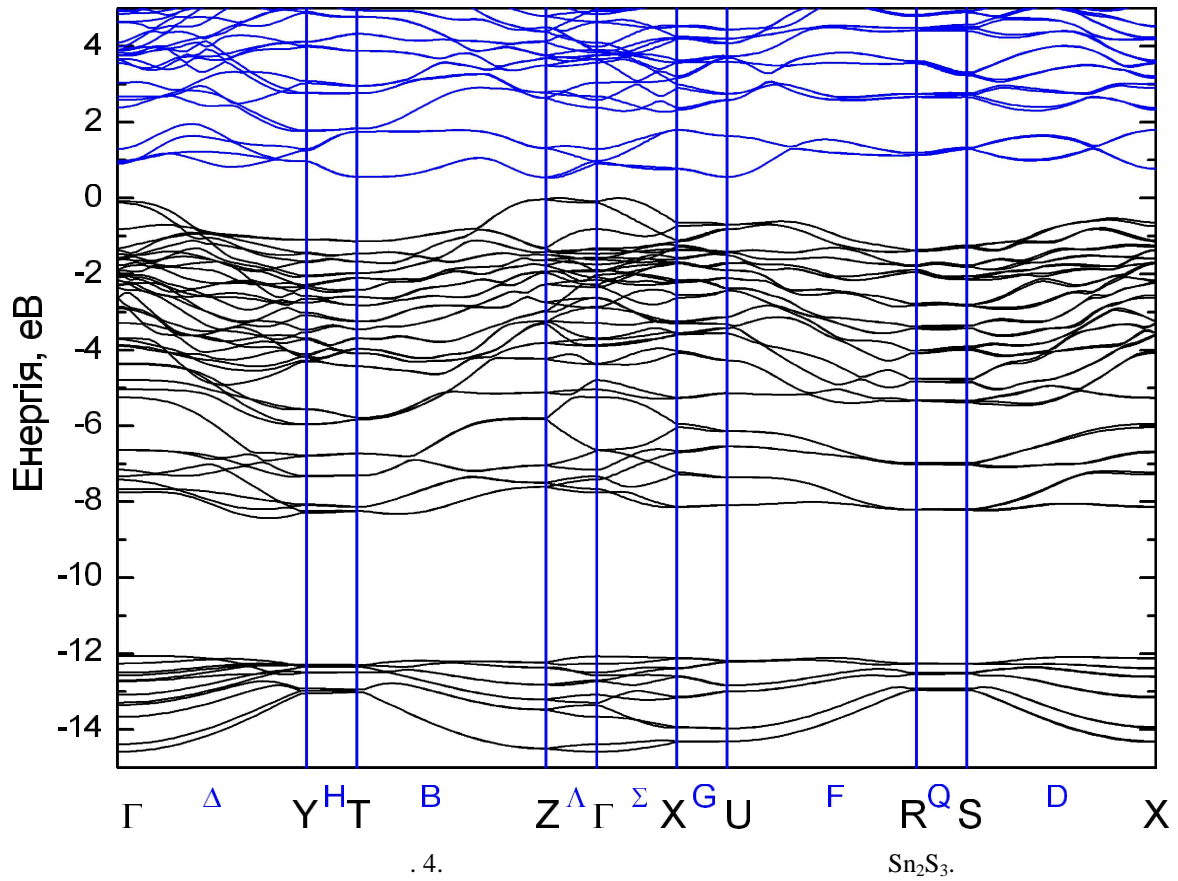
$h\nu = 1253.6$   
 $S3$  -  
 . 6  $S3p$

[7].  $\text{Sn}_2\text{S}_3$ , K-

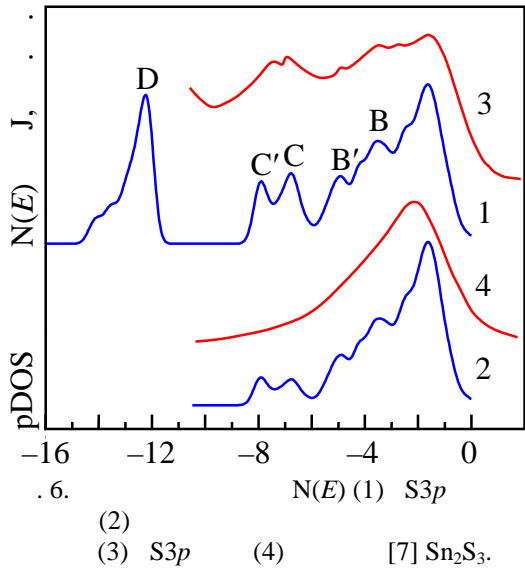
. 5, D  
 $\text{Sn}_2\text{S}_3$

3s- 3p-  
 5s- 3p- 5 -

3p- 3p-  
 5p- 5s-



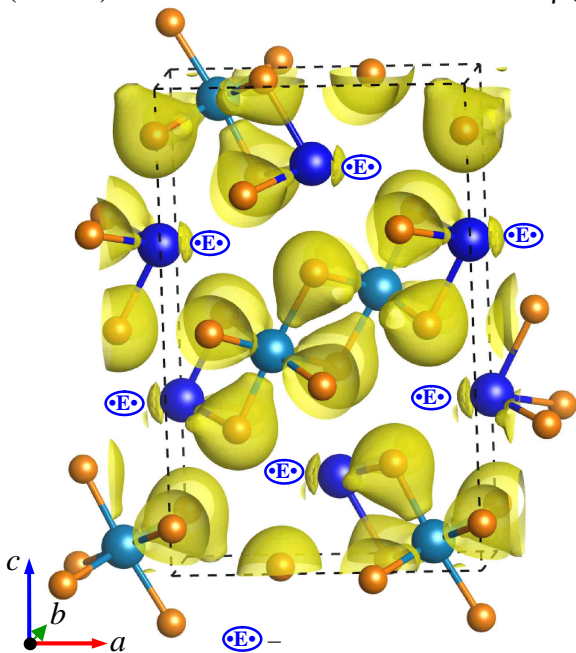
. 5.



3.3.



(. 7).



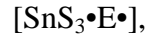
. 7.



. 7



$\psi^-$



$\rho(r)$

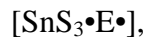
Sn-S.



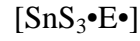
. 8



$\psi^-$



$\psi^-$



Sn-S



(. 7, 8).

S Sn -



Sn

+2 +4, S - +6,

*ab initio*



$E_{gi} = 0.53$

(  $\rightarrow U$ ).

$N(E)$

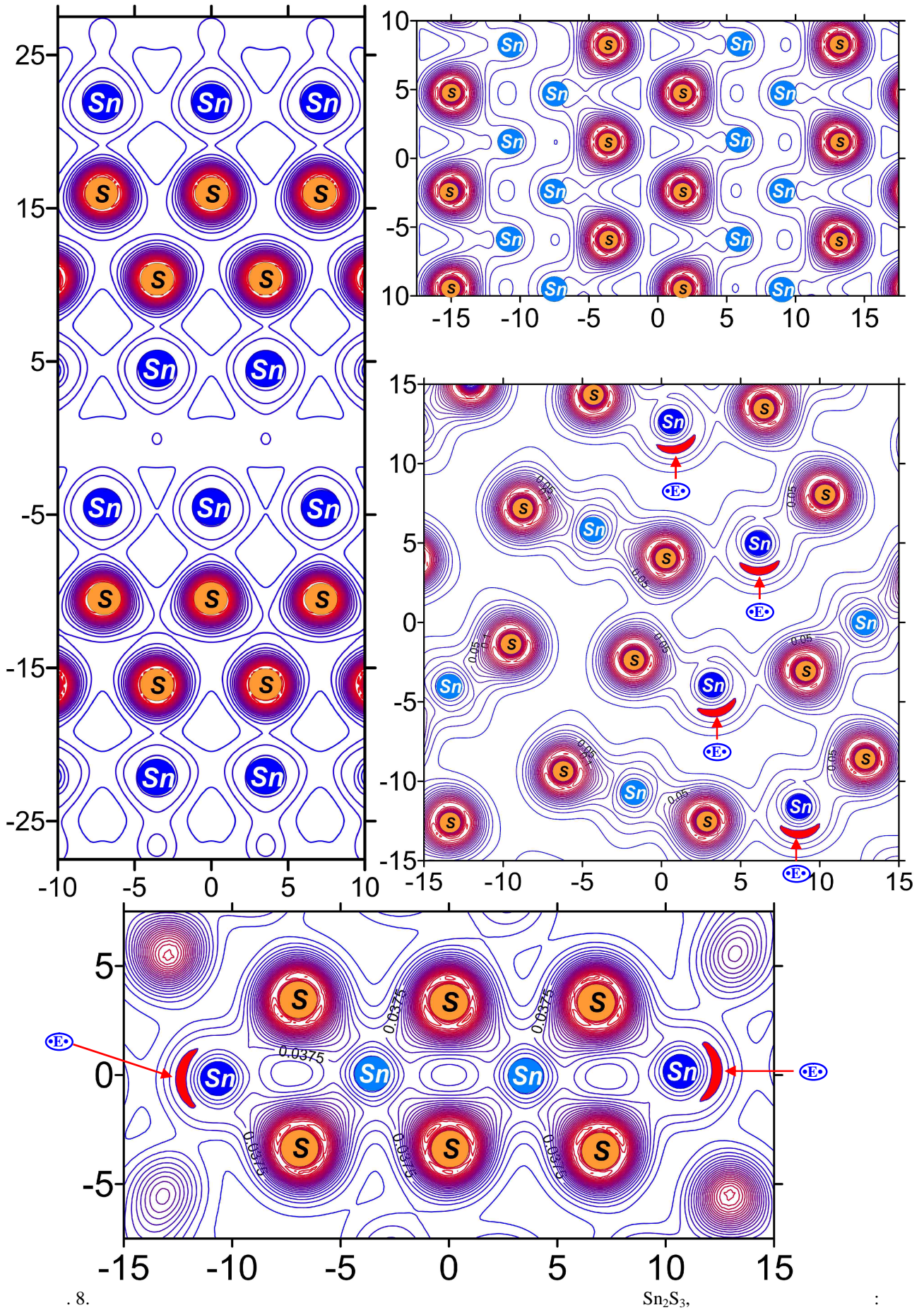
S3p-



2D 3D







. 8.

$-(100), -(001), -(010), -$   
68

1. ... ..  
// ... ..  
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20. ... ..  
... .., 1981. –  
420 .

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## ELECTRONIC STRUCTURE OF $\text{Sn}_2\text{S}_3$

The energy band structure, the spectra of total and local partial densities of states for  $\text{Sn}_2\text{S}_3$  crystal are calculated within the density functional theory. On the base of these results a detailed analysis of the valence states is performed. It is established that  $\text{Sn}_2\text{S}_3$  is an indirect-band semiconductor with the theoretically evaluated band gap of  $E_{\text{gi}} = 0.53$  eV. The calculated energy distributions of total and S3p partial densities of states are compared with known experimental X-ray photoelectron (XPS) and emission (XES) spectra. The electronic density maps in different planes are obtained, and the crystal can be characterized as an ion-covalent compound with the prevailing concentration of a charge on the S–Sn bonds in coordination  $\psi$ -tetrahedra and octahedra. It is revealed an important role of lone electronic pair in the formation of the  $\text{Sn}_2\text{S}_3$  atomic and electronic structures.

**Keywords:** tin sesquisulfide, electronic structure, density of states, lone pair.

• • • , • • • , 88000, • • • , 54

### $\text{Sn}_2\text{S}_3$

$\text{Sn}_2\text{S}_3$ ;

• • • • •  $\text{Sn}_2\text{S}_3$   $E_{\text{gi}} = 0.53$  S3p-  
 ( ) ( )  
 S–Sn  $\psi$ -  
 $\text{Sn}_2\text{S}_3$ .  
 ; , ,