

COMMUNICATION

T **d-** **L₂F₂SO₄**

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R 18 m 2015; m 4 D m 2015; 10 D m 2015
A 20 D m 2015

KEYWORDS

O₂ m
; d-O₂ m
; F
L₂F₂SO₄ m
L m

A. F. m (LIB) m m fi
. H, / mm
, m m
H, fi m m, (L O₄, F O₄)
O₄) L₂F₂SO₄ (l) F
m, d- “ ”
. M, (l) L -
F m, - L -

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LIB . F . m .

1 , 2 m - , $L_2M O_4$ ($M = F , C$) m .

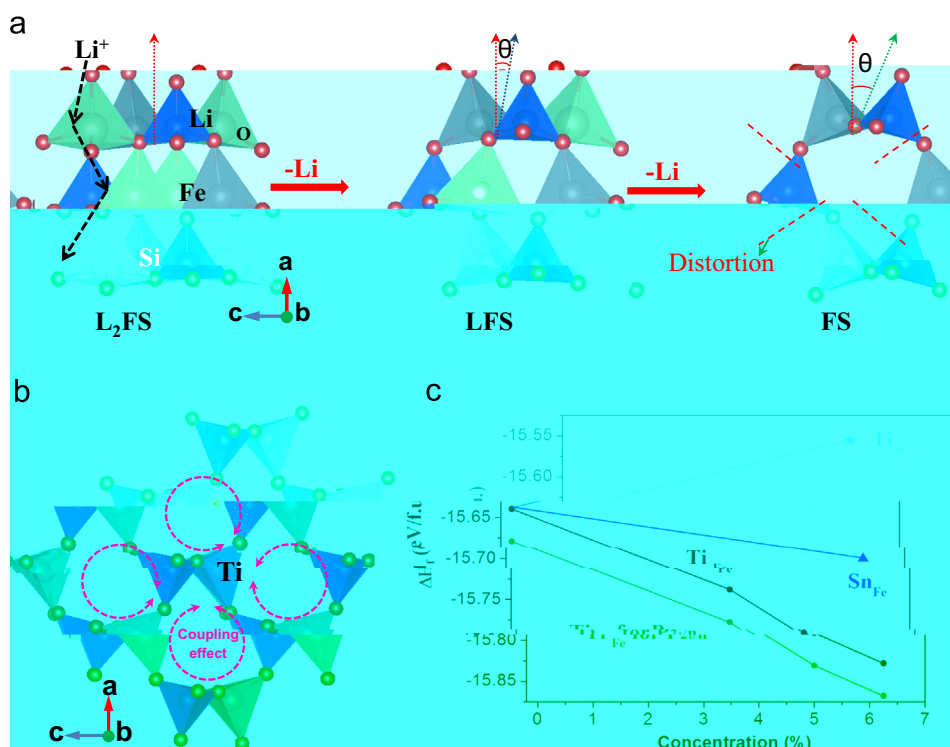
3 . A , m , m , m .

4 - , 6 .

7 .

LM $_2O_4$ 2 m , $L_2M O_4$ ($M = F , C$) LIB ? C m , m .

333 mA / . H , m .



F . 1 F - m . () F L - m .

L_2F , - ($L F O_4$ (LF)) m .

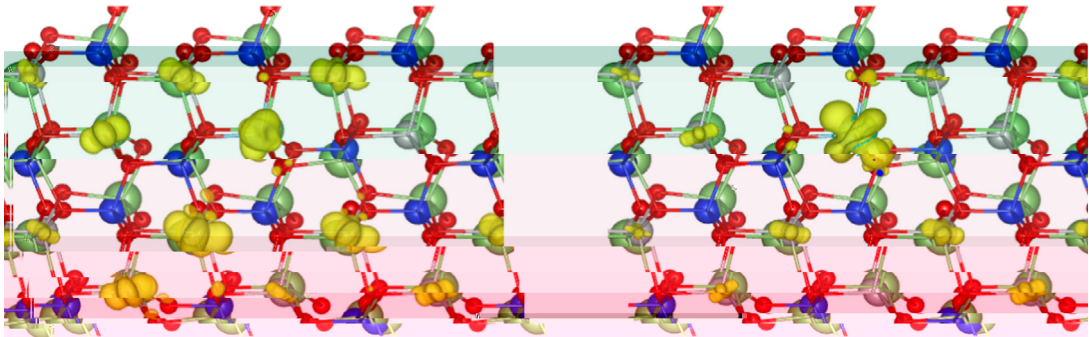
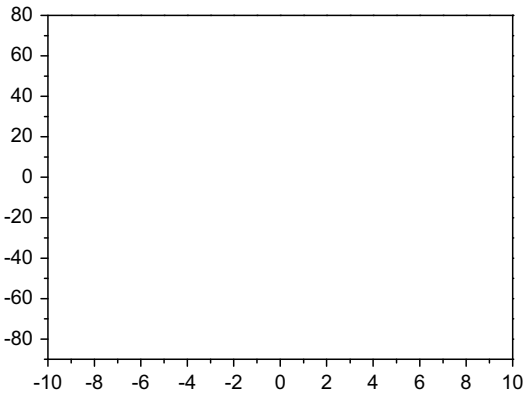
() F . E m .

($P2_1/$) , m .

$L_2F O_4$, F , m .

$P2_1$ $L_2F O_4$. (F)

$T = 1$	m	m	5%	-	L_2F	O_4	-	-
	()	()	()	(³)	ΔV ()			
L_2F	O_4	5.0228	5.4928	6.2675	172.915	0		
L	F	5.0813	5.2295	6.6996	178.028	2.96%		
F	O_4	5.3782	5.4174	7.4843	218.067	26.11%		
L_2F	$O_{0.095}$	5.0158	5.5028	6.2719	173.112	0		
L	$F_{0.095}$	5.0854	5.2163	6.7396	178.787	3.28%		
F	$O_{0.095}$	5.3828	5.4236	7.4919	218.728	26.35%		



H , m

O_4) L_2F O_4 m m , “ ” fi

(L O_4 , F O_4 O_4 L_2F O_4) m - M , (I)

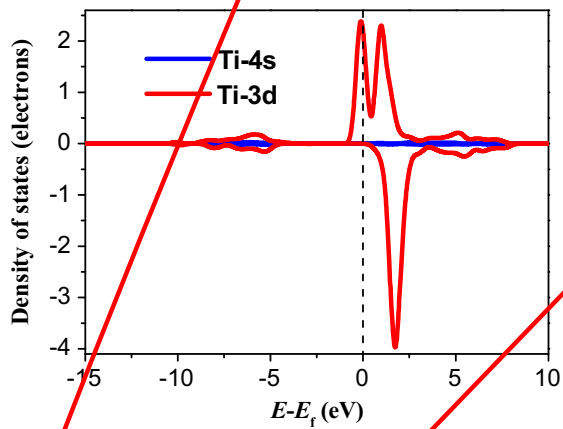
1 (F 1-10) 3 (F 17-19) m - . F , - L -

I . I m (I) L_2F O_4 , m . A m m fi m . A

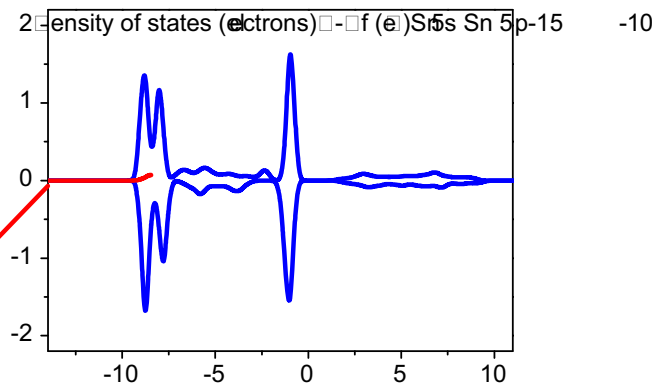
m) O (2) . (I) F (3 4 LIB .

C_{2v} $ab initio$ (PBE) (GGA) $PBE+U$ $U=4$ 5×10^{-6} $9 \times 9 \times 9$ $(2 \times 2 \times 1)$ 400

Ti	2	F	(ΔE_f)	$m_{x=0.0\%}$	(E_g)	$x=6.25\%$
	L_2F	O_4	3.75%	5%	6.25%	
ΔE_f	0	1.83	1.86	1.92		
E_g	2.13	1.68	1.46	1.50		



(NEB) m 12 m
 L_2F O_4
 DF m m 8 m m P $-B$
 $ab initio$ (PBE) 10 m
 E_m (GGA)
 $PBE+U$ 11 m $U=4$
 F_m 3 m m
 5×10^{-6} 0.01 $/$ m
 $9 \times 9 \times 9$ $(2 \times 2 \times 1)$ A m
 400
 $CH_3COOL \cdot 2H_2O$, 0.015 m 30 m $F(NO_3)_3 \cdot 9H_2O$, 0.03 m
 (EO) m m 20 m_L
 0.015 m
 $70^\circ C$ $80^\circ C$ 24 m 10
 $650^\circ C$ 10 m F m
 $L_2F_{1-x}xO_4$ $L_2F_{1-x}xO_4$ (B) (O_4)
 m m x A m
 fi m fi m m $(FE-EM, H)$
 $-4800, 10$ m $(HR EM, JEM-2100F, 200)$ m

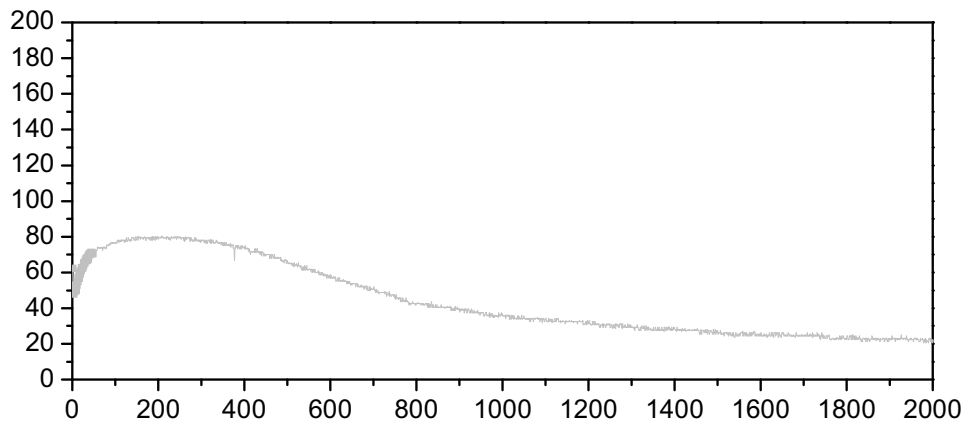


R

T

B m 5,13 , m
-L₂F O₄) (P2₁/
P^m₂₁)_m (F 11 20). H m
-P^m₂₁

S⁻
O (L O₄, F O₄ O₄ L₂F -
O₄) E
(-P^m₂₁),
L - . F 1 P^m₂₁ L₂F O₄ (L₂F), LF O₄ (LF),
F O₄ (F). I P^m₂₁ L₂F , L , F_m,
b,
- m . D L - , F O₄
F , O₄ m
(-O , F O₄
1.658 1.633). I O₄ m
. H , F O₄
m F O₄ O₄
fi b
. F 1 F O₄ O₄
θ *a* .
L - , θ ,
m m .
L : θ m m m , *a* *c*
7.1% 19.4%, , *b* 1.4%
L - (1). fi m
26.11% - m F O₄.
F O₄ O₄ fi
,
m m
m m
fi m ()
P2₁/ F . F 1



$\Delta H_f = E^{L_2F(1-x)} \times O_4 - 2E^L - (1-x)E^F$

$-xE^L - E^L - 2E^{O_2}$

$E^{L_2F(1-x)} \times O_4$

$O_4, E^L, E^F, E, E^{O_2}, L, F, L_2F, L - 19.45\%, L - (1), L_2F, O_4. A 4-6,$

$m, F, x, m, L - 0.82, P^{m_2} L_2F, O_4:$

$P^{m_2} L_1, L_2, L O_4 (L_2F$

$P^{m_2} L_1, F, F, F, L, c, a, L, m, L - 0.74, L_2F, O_4, m, L - El, fi-$

$(-O-(O-F-)) (F 1), F m, m, (F 13) (E_a) (F 14 4 I).$

$\Delta H_f.$

[illegible]

(F 5), L_2F O_4 , F 5 10 C-
 2000 . N , C-
 A , m . C m-
 LF 4, LF m-
 2000 m , m
 . F m , L_2F O_4 75%
 2000 , , fi L_2F O_4 (38%)
 L_2F O_4 N 33%, L_2F O_4 LF .
 E , m fi m
 L_2F O_4 m . H , L_2F O_4
 m , ~100% 2000

C -
 I mm , m fi
 m- m fi m L_2F O_4
 . m (-
), C- L_2F O_4 .
 m -
 m “ ” m ,
 (I) L_2F O_4 d-
 fi . L m d-
 L L
 L- . M L_2F O_4 m (I) m
 . m
 m m-
 m -

A-
 fi C (N . 51372186), N N
 E B (20121110, O m N ,), G -
 I m P (N . 2013N080),
 R G (N . D 20130331145131323,
 C 20120829172325895, JC J 20120614150338154, JC J
 20140903101633318).

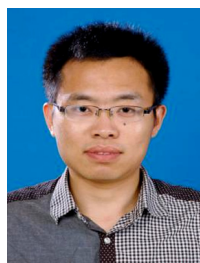
A

A. S

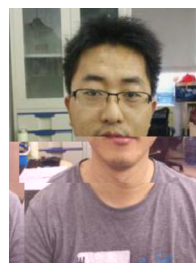
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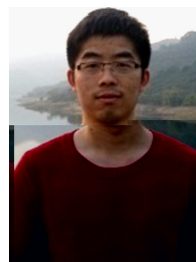
J. Y. A. J. P. D. B. 2008 m
 , C . m
 . H A G -
 , P , C m . H (m) ,
 : m , m .



K. W. N. M. M. B. 2013 m
 , C . H A
 , P , C m . H
 m



J. Z. P. D. B. 2008 P. D. 2013 m P.
 C. P. F. P. (AM), P. C. O. 2013 P. O. 2015. N. AM. H m
 : m , m , m
 m , m
 m), m



X. S. B. . P. 2013 M. , P. m
 A 2013, m m



X. K. P. B. 2011 m
 , C . M
 P . M
 K. L. M. A. P. M.
 : m 2014. H m



M. X. B. . P. 2011 m
 A. G. M. , P. C. M.
 m , m



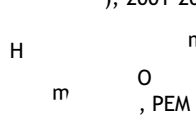
G. T. B. 2014. H. A. M. G.
 , P. C. m . H



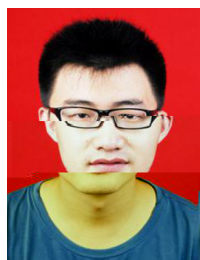
D. S. M. B. . P. D. 1995 m
 C. 2001. A. L. M. P. R. (F)



L. H. B. 2012 M. m
 2015 , C
 H : m



H. m O , PEM . H 2006 (2007-2008). H C m L m
 200



R. T. C. B. , C . H 2014
 A. M. M. , P , C
 H m , m



P. F. P. , D. A. M. , P. G. m , P. B. . m 1985
 P D m D . P&A C m , K, P . D. 1994. m P . P m
 . A C 150 m RMB
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2013.